# Fitting Analytical Surfaces to Points: General Approaches and Applications to Ellipsoid Fitting

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**Abstract:** A general solution methodology is presented for the problem of fitting an analytically described surface to a set of points by minimizing the sum of the squares of the minimal distances of the points from the surface. Two types of analytical representation of the surface are considered, the implicit representation where the surface is defined by a condition equation between the three Cartesian coordinates and the parametric one where the Cartesian coordinates are expressed as functions of two curvilinear coordinates on the surface. Both nonlinear system of equations defining the optimal solution, as well as approaches based on linearization and successive iterations are presented. The general results, which depend on the form of the surface representation (implicit or parametric), are then specialized to the specific case of the surface of a triaxial ellipsoid.

## 1. Introduction

The problem of best fitting of an analytical surface (i.e. a surface described by mathematical equations) to a given set of points has applications in many scientific fields, such as pattern recognition, particle physics, computer graphics, computer vision, CAD-CAM applications, virtual reality, robotics, medical imaging, structural geology, astronomy, metrology, photogrammetry and geodesy. Various methods have been presented in the literature, which differ mainly on how the distance of each point from the given surface is measured, while an optimal surface choice is the one where the distances of the given points are collectively minimized is some specific sense. Here we will examine least squares best fitting approaches where one minimizes the sum of the squares of the distances of a set of given points from their orthogonal projection on the relevant surface. We will determine the general system of nonlinear equations (nonlinear normal equations), which has as solution the optimal parameter estimates for two type of surface representations: the "implicit representation" where the surface is represented by a single equation in the three Cartesian coordinates and the "parametric representation" where the surface is represented by expressing the Cartesian coordinates of surface points as functions of two curvilinear surface coordinates. Following the geodetic–surveying tradition, we will also present corresponding iterative approaches based on the solution of the linearized least squares problem. Finally, the methods will be further elaborated by using the triaxial ellipsoid as an example of best fitting of a surface to a given set of points.

## 2. The problem of best fitting a surface to a given set of points as a mathematical constrained minimization problem

Let $\mathbf{x} = \begin{bmatrix} X & Y & Z \end{bmatrix}^T$ be the Cartesian coordinates of a point in three dimensions and let the surface $\pi$ under consideration be analytically represented by one of two forms, either by a single non-linear equation

(1) $$f(\mathbf{x},\mathbf{p}) = 0 ,$$

where $\mathbf{p} = \begin{bmatrix} p_1 & p_2 & \cdots & p_k \end{bmatrix}^T$ is the set of $k$ parameters defining the shape and position of the surface, or in the alternative parameterized form

(2) $$\mathbf{x} = \mathbf{x}(\mathbf{p},u,v) ,$$

where $u$ , $v$ is a pair of curvilinear coordinates on the surface. We will hereon call equation (1) the "implicit representation" and equation (2) the "parametric representation".

A very popular (mostly in the mathematical literature) but rather naive best fitting method is the algebraic method, where one minimizes the sum of squares of the "algebraic distances" (see e.g. Späth, 2001, Li & Griffiths, 2004, Markovsky, Kukush & Van Huffel, 2004, Bertoni, 2010, Malyugina, Andrews & Séquin, 2013, Igudesman & Chickrin, 2014), i.e., the residuals

(3) $$r_i = f(\mathbf{x}'_i,\mathbf{p}) \neq 0 ,$$

caused by the fact that a given set of $n$ points $\mathbf{x}'_i$, $i=1,2,...,n$, cannot exactly much the surface, or more precisely any of the surfaces within a family created by varying the values of the parameters defining its shape and its placement in space. Another type of distance is the "radial distance" which applies when the surface has a natural center with coordinates $\mathbf{c}$ . In this case the distance is between the point $\mathbf{x}'_i$ and the intersection $\mathbf{x}_i$ of the surface with the line joining the center $\mathbf{c}$ with the point $\mathbf{x}'_i$. Of course, the only distance worth of the characterization "best fitting" is the "orthogonal distance" between $\mathbf{x}'_i$ and its projection $\mathbf{x}_i$ on the surface, i.e. the closest point to $\mathbf{x}'_i$ among all surface points. There is an extensive literature on the so-called "geometric fitting" approach, see, e.g. Hu & Shrikhande (1995), Turner, Anderson, Mason & Cox (1999), Watson (2000), Ahn, Rauh, Cho & Warnecke (2002), Ahn, Rauh & Warnecke (2002), Ahn, Westkamper & Rauh (2002), Watson (2002), Atieg & Watson (2003), Ahn (2004), Liu & Wang (2008), Rouhani & Sappa (2009), Flory & Hofer (2010), Chernov & Ma (2011), Minh & Forbes (2012), Yu, Kulkarni & Poor (2012), Ruiz, Arroyave & Acosta (2013). The problem is typically solved by iterative techniques from optimization theory. We will follow here the geodesy-surveying tradition and in addition to the formulation of the nonlinear solution system (nonlinear normal equations) we will pursue iterative approaches which are based on model linearization and exploitation of the existing well-known solutions of linear least squares problems with the precautions pin-pointed out by Pope (1972).

Another aspect of the methodological diversity has to do with how all point distances are collectively taken into account, e.g. by minimizing the sum of their absolute values, or the sum of the squares of their absolute values (least squares approach) or the sum of some powers other that one and two (Watson, 2002, Helfrich & Zwick 2002).

Here we will consider only orthogonal or geometric distances and the least squares approach, where one minimizes the sum

$$\phi = \sum_{i=1}^{n} \| \mathbf{e}_i \|^2 = \sum_{i=1}^{n} \mathbf{e}_i^T \mathbf{e}_i = \sum_{i=1}^{n} (\mathbf{x}'_i - \mathbf{x}_i)^T (\mathbf{x}'_i - \mathbf{x}_i) = \min , \tag{4}$$

where $\mathbf{e}_i = \mathbf{x}'_i - \mathbf{x}_i$ is the vector joining each given point $\mathbf{x}'_i$ with its projection $\mathbf{x}_i$, and $\| \mathbf{e}_i \| = \sqrt{(\mathbf{x}'_i - \mathbf{x}_i)^T (\mathbf{x}'_i - \mathbf{x}_i)}$ is the corresponding magnitude or orthogonal distance. The above sum must be minimized under the condition that $\mathbf{x}_i$ are the projections on the surface of the corresponding given points $\mathbf{x}'_i$. This amounts to two mathematical conditions for each point, the condition $f(\mathbf{x}_i, \mathbf{p}) = 0$, which secures that the orthogonal projections lie on the surface and the projection (orthogonality) conditions $\mathbf{e}_i = \mathbf{x}'_i - \mathbf{x}_i \perp \pi$. To find the orthogonality conditions for the implicit representation approach, we need the gradient

$$\mathbf{g} = grad f = \left( \frac{\partial f}{\partial \mathbf{x}} \right)^T = \left[ \frac{\partial f}{\partial X} \quad \frac{\partial f}{\partial Y} \quad \frac{\partial f}{\partial Z} \right]^T = \mathbf{g}(\mathbf{x}, \mathbf{p}) , \tag{5}$$

which is a vector perpendicular to the surface $f(\mathbf{x}, \mathbf{p}) = 0$ and the requirement that $\mathbf{g}_i = \mathbf{g}(\mathbf{x}_i, \mathbf{p})$ is collinear with $\mathbf{e}_i = \mathbf{x}'_i - \mathbf{x}_i$. This can be easily expressed by three conditions per point, such as the vanishing of the exterior product $[\mathbf{g}_i \times] \mathbf{e}_i = \mathbf{0}$, or the equality $\frac{1}{|\mathbf{g}_i|} \mathbf{g}_i = \mathrm{sgn}(\mathbf{g}_i^T \mathbf{e}_i) \frac{1}{|\mathbf{e}_i|} \mathbf{e}_i$ of the corresponding unit vectors along $\mathbf{g}_i$ and $\mathbf{e}_i$. In both cases, the three conditions per point are superfluous and only two of them must be used, because the position of a point on a surface is defined by only two parameters. The strong nonlinearity of the equality of the unit vector approach leads to quite complicated relations and is therefore not worth considering. The exterior product approach depends on which two out of the conditions

$$\begin{aligned} [\mathbf{g}_i \times] \mathbf{e}_i = [\mathbf{g}_i \times](\mathbf{x}'_i - \mathbf{x}_i) &= \begin{bmatrix} 0 & -g_{Zi} & g_{Yi} \\ g_{Zi} & 0 & -g_{Xi} \\ -g_{Yi} & g_{Xi} & 0 \end{bmatrix} \begin{bmatrix} X'_i - X_i \\ Y'_i - Y_i \\ Z'_i - Z_i \end{bmatrix} = \\ &= \begin{bmatrix} -g_{Zi}(Y'_i - Y_i) + g_{Yi}(Z'_i - Z_i) \\ g_{Zi}(X'_i - X_i) - g_{Xi}(Z'_i - Z_i) \\ -g_{Yi}(X'_i - X_i) + g_{Xi}(Y'_i - Y_i) \end{bmatrix} = 0 , \end{aligned} \tag{6}$$

is taken into account. For a more appropriate set of conditions, note that if $\mathbf{e}_i = \mathbf{x}'_i - \mathbf{x}_i$ is collinear with $\mathbf{g}_i$, the first will be a scalar multiple of the second

(7) $$\mathbf{e}_i = \mathbf{x}'_i - \mathbf{x}_i = \rho_i \mathbf{g}_i ,$$

where $\rho_i$, $i = 1,2,...,n$, are additional unknowns, which counterbalance the use of three conditions in (7) instead of the only two required.

However, there is no need to implement any of these orthogonality conditions, neither two out of (6), nor (7). To understand this, consider the minimum $\min\limits_{\mathbf{p},\{\mathbf{x}_i\}} \phi$ of the target function $\phi(\mathbf{p}, \mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n)$ with respect to the unknown parameters $\mathbf{p}$ and $\{\mathbf{x}_i\}$, $i = 1,...,n$, as a two-step minimum $\min\limits_{\mathbf{p}} \{\min\limits_{\{\mathbf{x}_i\}} \phi\}$. In the first step a value of $\mathbf{p}$ is held fixed and the corresponding optimal values $\{\mathbf{x}_i(\mathbf{p})\}$ are found. In the second step the procedure is repeated for all possible values of $\mathbf{p}$ to find the global minimum at $\hat{\mathbf{p}}$ and $\{\hat{\mathbf{x}}_i\} = \{\mathbf{x}_i(\hat{\mathbf{p}})\}$. In the first step the fixed values of $\mathbf{p}$ define a known ellipsoid with fixed shape and placement, so that the minimization $\min\limits_{\{\mathbf{x}_i\}} \phi$ simply finds the surface points $\mathbf{x}_i$ which are closest to the respective given points $\mathbf{x}'_i$, i.e. their projections on the fixed ellipsoid surface, and thus the orthogonality condition of $\mathbf{x}'_i - \mathbf{x}_i$ with respect to the ellipsoid surface is automatically fulfilled.

In the case of the parametric representation $\mathbf{x} = \mathbf{x}(\mathbf{p}, u, v)$ of the surface, consider the two vectors $\mathbf{x}_u = \frac{\partial \mathbf{x}}{\partial u} = \mathbf{x}_u(\mathbf{p}, u, v)$, $\mathbf{x}_v = \frac{\partial \mathbf{x}}{\partial v} = \mathbf{x}_v(\mathbf{p}, u, v)$, which are tangent to the surface. To secure that $\mathbf{x}$ is the projection on the surface of a given point $\mathbf{x}'$, the vector $\mathbf{e} = \mathbf{x}' - \mathbf{x}$ must be perpendicular to the surface or equivalently to the two tangent vectors $\mathbf{x}_u$ and $\mathbf{x}_v$ at $\mathbf{x}$. The requirement that $\mathbf{x}_u \perp \mathbf{e}$, $\mathbf{x}_v \perp \mathbf{e}$, is guaranteed by the vanishing of the scalar products

(8) $$\mathbf{x}_u^T \mathbf{e} = 0 , \qquad \mathbf{x}_v^T \mathbf{e} = 0 .$$

As in the case of the implicit representation, there is no need to implement these orthogonality conditions. Again the minimum $\min\limits_{\mathbf{p},\{u_i,v_i\}} \phi$ of the target function $\phi(\mathbf{p}, u_1, v_1, u_2, v_2, ..., u_n, v_n)$ with respect to the unknown parameters $\mathbf{p}$ and $\{u_i, v_i\}$, $i = 1,...,n$, may be viewed as a two-step minimum $\min\limits_{\mathbf{p}} \{\min\limits_{\{u_i,v_i\}} \phi\}$, where in the first step a value of $\mathbf{p}$ is held fixed defining a known ellipsoid with fixed shape and placement. The corresponding optimal values $\{u_i(\mathbf{p}), v_i(\mathbf{p})\}$ produce surface points $\mathbf{x}(u_i, v_i)$ which are closest to the respective given points $\mathbf{x}'_i$, i.e. their projections on the fixed ellipsoid surface. Thus the orthogonality condition of $\mathbf{x}'_i - \mathbf{x}(u_i, v_i)$ with respect to the ellipsoid surface is again automatically fulfilled.

We are now in a position to define the optimization problem of the best fitting surface in either of the two possible forms:

Implicit representation approach $f(\mathbf{x},\mathbf{p})=0$: We need to minimize

(9) $$\phi=\sum_{i=1}^{n}(\mathbf{x}_i'-\mathbf{x}_i)^T(\mathbf{x}_i'-\mathbf{x}_i)=\min,$$

subject to the constraints

(10) $$f(\mathbf{x}_i,\mathbf{p})=0, \quad i=1,2,\ldots,n.$$

In the above formulation we minimize a function of $3n+k$ unknowns ($3n$ for $\mathbf{x}_i$, $k$ for $\mathbf{p}$) subject to $n$ constraints. The difference unknowns minus conditions $(3n+k)-n=2n+k$ amounts to the actual number of unknowns since two parameters are sufficient to determine the position of each $\mathbf{x}_i$ on the particular surface.

Parametric representation approach $\mathbf{x}=\mathbf{x}(\mathbf{p},u,v)$: We need to minimize

(11) $$\phi=\sum_{i=1}^{n}(\mathbf{x}_i'-\mathbf{x}_i)^T(\mathbf{x}_i'-\mathbf{x}_i)=\sum_{i=1}^{n}[\mathbf{x}_i'-\mathbf{x}(\mathbf{p},u_i,v_i)]^T[\mathbf{x}_i'-\mathbf{x}(\mathbf{p},u_i,v_i)]=\min.$$

If one attempts to impose the two conditions

(12) $$\mathbf{x}_u(\mathbf{p},u_i,v_i)^T\left[\mathbf{x}_i'-\mathbf{x}(\mathbf{p},u_i,v_i)\right]=0,$$

(13) $$\mathbf{x}_v(\mathbf{p},u_i,v_i)^T\left[\mathbf{x}_i'-\mathbf{x}(\mathbf{p},u_i,v_i)\right]=0, \quad i=1,2,\ldots,n.$$

he will derive exactly the same solution as in the standard case where they are ignored. We leave the proof of this statement as an interesting exercise to the reader.

## 3. Nonlinear solution for the implicit representation approach

In order to solve the constrained minimization problem of equations (9), (10), we must form the Lagrangean

(14) $$\Phi=\sum_{i=1}^{n}(\mathbf{x}_i'-\mathbf{x}_i)^T(\mathbf{x}_i'-\mathbf{x}_i)-2\sum_{i=1}^{n}\lambda_i f(\mathbf{x}_i,\mathbf{p})$$

and set to zero its derivatives with respect to the unknowns $\mathbf{x}_i$, $\mathbf{p}$, as well as, with respect to the Lagrange multipliers $\lambda_i$, thus recovering the constraints as part of the solution system. Since

(15) $$\frac{\partial\Phi}{\partial\mathbf{x}_i}=-2(\mathbf{x}_i'-\mathbf{x}_i)^T-2\lambda_i\frac{\partial f}{\partial\mathbf{x}_i}(\mathbf{x}_i,\mathbf{p})=-2(\mathbf{x}_i'-\mathbf{x}_i)^T-2\lambda_i\,\mathbf{g}(\mathbf{x}_i,\mathbf{p})^T=0,$$

(16) $$\frac{\partial\Phi}{\partial\mathbf{p}}=-2\sum_{i=1}^{n}\lambda_i\frac{\partial f}{\partial\mathbf{p}}(\mathbf{x}_i,\mathbf{p})\equiv-2\sum_{i=1}^{n}\lambda_i\mathbf{z}(\mathbf{x}_i,\mathbf{p})^T=\mathbf{0},$$

(17) $$\frac{\partial\Phi}{\partial\lambda_i} = -2f(\mathbf{x}_i,\mathbf{p}) = 0$$

where

(18) $$\mathbf{g}_i = \left(\frac{\partial f}{\partial\mathbf{x}}\right)^T(\mathbf{x}_i,\mathbf{p}) = \mathbf{g}(\mathbf{x}_i,\mathbf{p}),$$

(19) $$\mathbf{z}_i = \left(\frac{\partial f}{\partial\mathbf{p}}\right)^T(\mathbf{x}_i,\mathbf{p}) = \mathbf{z}(\mathbf{x}_i,\mathbf{p}),$$

the solution $\hat{\mathbf{x}}_i$, $\hat{\mathbf{p}}$, $\hat{\lambda}_i$ is provided by the "nonlinear normal equations"

(20) $$\mathbf{x}'_i - \mathbf{x}_i + \lambda_i\,\mathbf{g}(\mathbf{x}_i,\mathbf{p}) = \mathbf{0}, \qquad i = 1,2,...,n,$$

(21) $$\sum_{i=1}^{n}\lambda_i\,\mathbf{z}(\mathbf{x}_i,\mathbf{p}) = \mathbf{0},$$

(22) $$f(\hat{\mathbf{x}}_i,\hat{\mathbf{p}}) = 0, \qquad i = 1,2,...,n.$$

It is interesting to notice that although the orthogonality condition of $\mathbf{x}'_i - \mathbf{x}_i$ to the surface, as guaranteed by its collinearity (7) with the perpendicular to the surface gradient vector $\mathbf{g}(\mathbf{x}_i,\mathbf{p})$, has not been directly implemented, it results as part of the solution system (equation 20) and thus $\mathbf{x}'_i - \mathbf{x}_i$ is indeed perpendicular to the surface as required.

These equations can be solved either by various iteration schemes, as they stand or after elimination of some of the unknowns. The specific solution method strongly depends on the specific form of the surface representation equation $f(\mathbf{x},\mathbf{p}) = 0$. When good approximate values $\mathbf{x}_0$ are known for the unknown parameters in the above nonlinear equations of the form $\mathbf{f}(\mathbf{x}) = \mathbf{0}$, an iteration scheme can be based on the linearization by Taylor expansion retaining only first order terms in $\delta\mathbf{x} = \mathbf{x} - \mathbf{x}_0$. Thus $\mathbf{f}(\mathbf{x}) \approx \mathbf{f}(\mathbf{x}_0) + \frac{\partial\mathbf{f}}{\partial\mathbf{x}}(\mathbf{x}_0)\delta\mathbf{x} \equiv \mathbf{f}_0 + \mathbf{J}\delta\mathbf{x} = \mathbf{0}$, and since the Jacobean matrix is nonsingular in general, $\delta\hat{\mathbf{x}} = -\mathbf{J}^{-1}\mathbf{f}_0$. The estimates $\hat{\mathbf{x}} = \mathbf{x}_0 + \delta\hat{\mathbf{x}} = \\ = \mathbf{x}_0 - \mathbf{J}^{-1}\mathbf{f}_0$ are the used as approximate values for the next iteration step and so on, until convergence is achieved. This is the well-known Newton's iterative solution (see, e.g. Nocedal & Wright, 1999, Ortega & Rheinboldt, 2000).

## 4. Solution with linearization and iterations for the implicit representation approach

A typical approach in geodesy and surveying for treating nonlinear least squares problems is the linearization of the relevant models, the exploitation of the corresponding linear problem solution, and its further improvement through iterations (Pope, 1972). Since the data $\mathbf{x}'_i$ are already linear in the unknowns $\mathbf{x}_i$ ($\mathbf{x}'_i = \mathbf{x}_i + \mathbf{e}_i$), we only need to linearize the nonlinear constraints using approximate values $\mathbf{x}_{i0}$, $\mathbf{p}_0$ for the unknowns $\mathbf{x}_i = \mathbf{x}_{i0} + \delta\mathbf{x}_i$, $\mathbf{p} = \mathbf{p}_0 + \delta\mathbf{p}$. In fact we only need to find the approximate values $\mathbf{p}_0$, e.g. by the relatively easy solution of the algebraic method (see below). The values $\mathbf{x}_{i0}$ may be found by projecting the data points $\mathbf{x}'_i$ on the approximate surface defined by the $\mathbf{p}_0$ (see e.g. the approach proposed in appendix A). In such a case it will hold that $f(\mathbf{x}_{i0}, \mathbf{p}_0) = 0$, but for the sake of generality we will make no use of this simplification. The required linearizations are

(23) $$f(\mathbf{x}_i, \mathbf{p}) = f(\mathbf{x}_{i0}, \mathbf{p}_0) + \left(\frac{\partial f}{\partial \mathbf{x}_i}\right)_0 \delta\mathbf{x}_i + \left(\frac{\partial f}{\partial \mathbf{p}}\right)_0 \delta\mathbf{p} = f_{i0} + \mathbf{g}_{i0}^T \delta\mathbf{x}_i + \mathbf{z}_{i0}^T \delta\mathbf{p} = 0,$$
$$i = 1, 2, \ldots, n,$$

where $f_{i0} = f(\mathbf{x}_{i0}, \mathbf{p}_0)$, $\mathbf{g}_{i0} = \mathbf{g}(\mathbf{x}_{i0}, \mathbf{p}_0)$, $\mathbf{z}_{i0} = \mathbf{z}(\mathbf{x}_{i0}, \mathbf{p}_0)$. The "observation" equations $\mathbf{x}'_i = \mathbf{x}_i + \mathbf{e}_i$ take the linearized form

(24) $$\mathbf{b}_i \equiv \mathbf{x}'_i - \mathbf{x}_{i0} = \delta\mathbf{x}_i + \mathbf{e}_i, \qquad i = 1, 2, \ldots, n.$$

For all points $i = 1, 2, \ldots, n$ the observation equations become

(25) $$\mathbf{b} \equiv \begin{bmatrix} \mathbf{x}'_1 - \mathbf{x}_{10} \\ \vdots \\ \mathbf{x}'_n - \mathbf{x}_{n0} \end{bmatrix} = \begin{bmatrix} \delta\mathbf{x}_1 \\ \vdots \\ \delta\mathbf{x}_n \end{bmatrix} + \begin{bmatrix} \mathbf{e}_1 \\ \vdots \\ \mathbf{e}_n \end{bmatrix} \equiv \delta\mathbf{x} + \mathbf{e},$$

while the constraints become

(26) $$\begin{bmatrix} f_{10} \\ \vdots \\ f_{n0} \end{bmatrix} + \begin{bmatrix} \mathbf{g}_{10}^T & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \mathbf{g}_{n0}^T \end{bmatrix} \begin{bmatrix} \delta\mathbf{x}_1 \\ \vdots \\ \delta\mathbf{x}_n \end{bmatrix} + \begin{bmatrix} \mathbf{z}_{10}^T \\ \vdots \\ \mathbf{z}_{n0}^T \end{bmatrix} \delta\mathbf{p} \equiv \mathbf{f}_0 + \mathbf{G}^T \delta\mathbf{x} + \mathbf{Z}\delta\mathbf{p} = \mathbf{0}.$$

This has the form of a least squares problem $\mathbf{b} = \mathbf{A}\mathbf{x} + \mathbf{e}$, $\mathbf{e}^T\mathbf{P}\mathbf{e} = \min$, with constraints $\mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{y} + \mathbf{d} = \mathbf{0}$, which differ from the standard well-known "observations equations with linear constraints" case, because the constraints contain additional parameters $\mathbf{y}$ not present in the observation equations. The required solution is derived in appendix B, and the relevant equations (B10) and (B11), take in our specific case, where $\mathbf{P} = \mathbf{I}$, $\mathbf{A} = \mathbf{I}$ and thus $\mathbf{N} = \mathbf{I}$, $\mathbf{u} = \mathbf{b}$, the simplified form

(27) $$\hat{\mathbf{y}} = -\left[\mathbf{D}^T (\mathbf{C}\mathbf{C}^T)^{-1} \mathbf{D}\right]^{-1} \mathbf{D}^T (\mathbf{C}\mathbf{C}^T)^{-1} (\mathbf{C}\mathbf{b} + \mathbf{d}).$$

(28) $$\hat{\mathbf{x}} = \mathbf{b} - \mathbf{C}^T (\mathbf{C}\mathbf{C}^T)^{-1} (\mathbf{C}\mathbf{b} + \mathbf{d}) - \mathbf{C}^T (\mathbf{C}\mathbf{C}^T)^{-1} \mathbf{D}\hat{\mathbf{y}}.$$

Applying the above equations with $\mathbf{C} \to \mathbf{G}^T$, $\mathbf{D} \to \mathbf{Z}$, $\mathbf{d} \to \mathbf{f}_0$, $\hat{\mathbf{x}} \to \delta\hat{\mathbf{x}}$, $\mathbf{y} \to \delta\hat{\mathbf{p}}$, gives the desired solution

(29) $$\delta\hat{\mathbf{p}} = -\left[\mathbf{Z}^T(\mathbf{G}^T\mathbf{G})^{-1}\mathbf{Z}\right]^{-1}\mathbf{Z}^T(\mathbf{G}^T\mathbf{G})^{-1}(\mathbf{G}^T\mathbf{b} + \mathbf{f}_0) .$$

(30) $$\delta\hat{\mathbf{x}} = \mathbf{b} - \mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1}(\mathbf{G}^T\mathbf{b} + \mathbf{f}_0) - \mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1}\mathbf{Z}\delta\hat{\mathbf{p}} .$$

Setting

(31) $$\kappa_{i0} = \mathbf{g}_{i0}^T\mathbf{g}_{i0} , \qquad i = 1,\dots,n ,$$

it is easy to show that

(32) $$(\mathbf{G}^T\mathbf{G})^{-1} = \begin{bmatrix} \frac{1}{\kappa_{10}} & \cdots & \mathbf{0} \\ \vdots & \ddots & \vdots \\ \mathbf{0} & \cdots & \frac{1}{\kappa_{n0}} \end{bmatrix},$$

(33) $$\mathbf{G}^T\mathbf{b} + \mathbf{f}_0 = \begin{bmatrix} \mathbf{g}_{10}^T(\mathbf{x}_1' - \mathbf{x}_{10}) + f_{10} \\ \vdots \\ \mathbf{g}_{n0}^T(\mathbf{x}_n' - \mathbf{x}_{n0}) + f_{n0} \end{bmatrix},$$

(34) $$\mathbf{Z}^T(\mathbf{G}^T\mathbf{G})^{-1} = \begin{bmatrix} \frac{1}{\kappa_{10}}\mathbf{z}_{01} & \cdots & \frac{1}{\kappa_{n0}}\mathbf{z}_{0n} \end{bmatrix},$$

(35) $$\mathbf{Z}^T(\mathbf{G}^T\mathbf{G})^{-1}\mathbf{Z} = \sum_{i=1}^{n}\frac{1}{\kappa_{10}}\mathbf{z}_{0i}\mathbf{z}_{i0}^T ,$$

and the solution (29), (30) takes the explicit form

(36) $$\delta\hat{\mathbf{p}} = -\left(\sum_{i=1}^{n}\frac{1}{\kappa_{i0}}\mathbf{z}_{0i}\mathbf{z}_{i0}^T\right)^{-1}\left(\sum_{i=1}^{n}\frac{\mathbf{g}_{i0}^T(\mathbf{x}_i' - \mathbf{x}_{i0}) + f_{i0}}{\kappa_{i0}}\mathbf{z}_{0i}\right),$$

(37) $$\delta\hat{\mathbf{x}}_i = \mathbf{x}_i' - \mathbf{x}_{i0} - \frac{\mathbf{g}_{i0}^T(\mathbf{x}_i' - \mathbf{x}_{i0}) + f_{i0}}{\kappa_{i0}}\mathbf{g}_{i0} - \frac{1}{\kappa_{i0}}\mathbf{g}_{i0}\mathbf{z}_{i0}^T\delta\hat{\mathbf{p}} .$$

The estimates $\hat{\mathbf{x}}_i = \mathbf{x}_{i0} + \delta\hat{\mathbf{x}}_i$, $\hat{\mathbf{p}} = \mathbf{p}_0 + \delta\hat{\mathbf{p}}$ are the approximate values for the next iteration step, until convergence is achieved. We may also use only equation (36) to obtain $\hat{\mathbf{p}} = \mathbf{p}_0 + \delta\hat{\mathbf{p}}$ and retrieve instead the estimates $\hat{\mathbf{x}}_i$ by projecting each $\mathbf{x}_i'$ on the ellipsoid defined by $\hat{\mathbf{p}}$ using any projection algorithm (see e.g. the proposed approach in appendix A).

## 5. Nonlinear solution for the parametric representation approach

The minimization problem to be solved in this case is defined by equation (11) and has target function

(38) $$\phi = \sum_{i=1}^{n} [\mathbf{x}'_i - \mathbf{x}(\mathbf{p}, u_i, v_i)]^T [\mathbf{x}'_i - \mathbf{x}(\mathbf{p}, u_i, v_i)] = \min_{\mathbf{p},\{u_i, v_i\}} .$$

Setting the derivatives of $\phi$ with respect to the unknowns equal to zero, using the subscripts $u$, $v$ to denote partial derivatives of $\mathbf{x}(\mathbf{p}, u, v)$ with respect to these parameters, e.g. $\mathbf{x}_u = \partial \mathbf{x} / \partial u$, $\mathbf{x}_v = \partial \mathbf{x} / \partial v$, $\mathbf{x}_p = \partial \mathbf{x} / \partial \mathbf{p}$ , etc., and the subscript $i$ to denote evaluation for $u_i$, $v_i$, we have

(39) $$\frac{\partial \phi}{\partial u_i} = -2(\mathbf{x}'_i - \mathbf{x}_i)^T \frac{\partial \mathbf{x}}{\partial u_i} = -2(\mathbf{x}'_i - \mathbf{x}_i)^T \mathbf{x}_{ui} = 0 , \qquad i = 1, 2, ..., n ,$$

(40) $$\frac{\partial \phi}{\partial v_i} = -2(\mathbf{x}'_i - \mathbf{x}_i)^T \frac{\partial \mathbf{x}}{\partial v_i} = -2(\mathbf{x}'_i - \mathbf{x}_i)^T \mathbf{x}_{vi} = 0 , \qquad i = 1, 2, ..., n ,$$

(41) $$\frac{\partial \phi}{\partial \mathbf{p}} = -2\sum_{i=1}^{n} (\mathbf{x}'_i - \mathbf{x}_i)^T \frac{\partial \mathbf{x}_i}{\partial \mathbf{p}} = -2\sum_{i=1}^{n} (\mathbf{x}'_i - \mathbf{x}_i)^T \mathbf{x}_{pi} = \mathbf{0} .$$

Therefore the system of nonlinear equations (nonlinear normal equations) to be solved is

(42) $$\sum_{i=1}^{n} (\mathbf{x}_{pi}^T \mathbf{x}'_i - \mathbf{x}_{pi}^T \mathbf{x}_i) = 0 ,$$

(43) $$\mathbf{x}_{ui}^T (\mathbf{x}'_i - \mathbf{x}_i) = 0 , \quad i = 1, 2, ..., n ,$$

(44) $$\mathbf{x}_{vi}^T (\mathbf{x}'_i - \mathbf{x}_i) = 0 , \quad i = 1, 2, ..., n .$$

It is interesting to notice that although the orthogonality conditions (12), (13) have not been directly implemented, they result as part of the solution system (equations 43 and 44) and thus $\mathbf{x}'_i - \mathbf{x}_i$ is indeed perpendicular to the surface as required.

In order to write the solution system in a more compact way we introduce the new functions

(45) $$\beta_u = \mathbf{x}^T \mathbf{x}_u , \qquad \beta_v = \mathbf{x}^T \mathbf{x}_v ,$$

(46) $$\varepsilon_u = \mathbf{x}'^T \mathbf{x}_u , \qquad \varepsilon_v = \mathbf{x}'^T \mathbf{x}_v ,$$

(47) $$\mathbf{b}_p = \mathbf{x}_p^T \mathbf{x} , \qquad \mathbf{e}_p = \mathbf{x}_p^T \mathbf{x}' .$$

In terms of the above functions the solution system for the unknowns $u_i$, $v_i$ , $\mathbf{p}$ takes the form

(48) $$\sum_{i=1}^{n} \mathbf{e}_p(\mathbf{x}'_i, \mathbf{p}, u_i, v_i) = \sum_{i=1}^{n} \mathbf{b}_p(\mathbf{p}, u_i, v_i) ,$$

(49) $$\varepsilon_u(\mathbf{x}'_i,\mathbf{p},u_i,v_i)=\beta_u(\mathbf{p},u_i,v_i)\,,\qquad i=1,2,\ldots,n\,,$$

(50) $$\varepsilon_v(\mathbf{x}'_i,\mathbf{p},u_i,v_i)=\beta_v(\mathbf{p},u_i,v_i)\,,\qquad i=1,2,\ldots,n\,,$$

which is a system of $k+n+n=2n+k$ nonlinear equations in the $2n+k$ unknowns $u_i$, $v_i$ and $\mathbf{p}$. Further development depends on the specific form of the function $\mathbf{x}(u,v,\mathbf{p})$ from which the forms of the functions defined above derive, and on the choice of a particular solution method.

## 6. Solution with linearization and iterations for the parametric representation approach

The nonlinear observation equation in the case of the parametric representation is

(51) $$\mathbf{x}'_i=\mathbf{x}(\mathbf{p},u_i,v_i)+\mathbf{e}_i\,.$$

We shall denote with subscripts derivatives with respect to the corresponding parameters, e.g. $\mathbf{x}_u=\partial\mathbf{x}/\partial u$, $\mathbf{x}_v=\partial\mathbf{x}/\partial v$, $\mathbf{x}_p=\partial\mathbf{x}/\partial\mathbf{p}$, etc., while an additional subscript "$i0$" denotes evaluation at known approximate values $u_{i0}$, $v_{i0}$, e.g. $\mathbf{x}_{i0}=\mathbf{x}(u_{i0},v_{i0})$, $\mathbf{x}_{u,i0}=\mathbf{x}_u(u_{i0},v_{i0})$, $\mathbf{x}_{v,i0}=\mathbf{x}_v(u_{i0},v_{i0})$, etc. Linearization by Taylor expansion retaining only first order terms, with $u_i=u_{i0}+\delta u_i$, $v_i=v_{i0}+\delta v_i$, gives

(52) $$\mathbf{x}(\mathbf{p},u_i,v_i)=\mathbf{x}_{i0}+\mathbf{x}_{p,i0}\delta\mathbf{p}+\mathbf{x}_{u,i0}\delta u_i+\mathbf{x}_{v,i0}\delta v_i\,,$$

The observation equations take the linearized form

$$\mathbf{x}'_i=\mathbf{x}_{i0}+\mathbf{x}_{p,i0}\delta\mathbf{p}+\mathbf{x}_{u,i0}\delta u_i+\mathbf{x}_{v,i0}\delta v_i+\mathbf{e}_i$$

or

(53) $$\mathbf{x}'_i-\mathbf{x}_{i0}=\mathbf{x}_{p,i0}\delta\mathbf{p}+\mathbf{x}_{u,i0}\delta u_i+\mathbf{x}_{v,i0}\delta v_i+\mathbf{e}_i\,.$$

For all points $i=1,2,\ldots,n$ the linearized observation equations are

(54) $$\mathbf{b}\equiv\begin{bmatrix}\mathbf{x}'_1-\mathbf{x}_{10}\\ \vdots\\ \mathbf{x}'_n-\mathbf{x}_{n0}\end{bmatrix}=\begin{bmatrix}\mathbf{x}_{p,10}\\ \vdots\\ \mathbf{x}_{p,n0}\end{bmatrix}\delta\mathbf{p}+\begin{bmatrix}\mathbf{x}_{u,10} & \cdots & 0\\ \vdots & \ddots & \vdots\\ 0 & \cdots & \mathbf{x}_{u,n0}\end{bmatrix}\begin{bmatrix}\delta u_1\\ \vdots\\ \delta u_n\end{bmatrix}+$$

$$+\begin{bmatrix}\mathbf{x}_{v,10} & \cdots & 0\\ \vdots & \ddots & \vdots\\ 0 & \cdots & \mathbf{x}_{v,n0}\end{bmatrix}\begin{bmatrix}\delta v_1\\ \vdots\\ \delta v_n\end{bmatrix}+\begin{bmatrix}\mathbf{e}_1\\ \vdots\\ \mathbf{e}_n\end{bmatrix}\equiv$$

$$\equiv\mathbf{A}_p\delta\mathbf{p}+\mathbf{A}_u\delta\mathbf{u}+\mathbf{A}_v\delta\mathbf{v}+\mathbf{e}=\begin{bmatrix}\mathbf{A}_p & \mathbf{A}_u & \mathbf{A}_v\end{bmatrix}\begin{bmatrix}\delta\mathbf{p}\\ \delta\mathbf{u}\\ \delta\mathbf{v}\end{bmatrix}+\mathbf{e}=\mathbf{A}\mathbf{x}+\mathbf{e}\,.$$

The normal equations are $\mathbf{N}\hat{\mathbf{x}} = \mathbf{u}$ with

(55) $$\mathbf{N} = \begin{bmatrix} \mathbf{A}_p^T\mathbf{A}_p & \mathbf{A}_p^T\mathbf{A}_u & \mathbf{A}_p^T\mathbf{A}_v \\ \mathbf{A}_u^T\mathbf{A}_p & \mathbf{A}_u^T\mathbf{A}_u & \mathbf{A}_u^T\mathbf{A}_v \\ \mathbf{A}_v^T\mathbf{A}_p & \mathbf{A}_v^T\mathbf{A}_u & \mathbf{A}_v^T\mathbf{A}_v \end{bmatrix} \equiv \begin{bmatrix} \mathbf{N}_p & \mathbf{N}_{pu} & \mathbf{N}_{pv} \\ \mathbf{N}_{pu}^T & \mathbf{N}_u & \mathbf{N}_{uv} \\ \mathbf{N}_{pv}^T & \mathbf{N}_{uv}^T & \mathbf{N}_v \end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix} \mathbf{A}_p^T\mathbf{b} \\ \mathbf{A}_u^T\mathbf{b} \\ \mathbf{A}_v^T\mathbf{b} \end{bmatrix} \equiv \begin{bmatrix} \mathbf{u}_p \\ \mathbf{u}_u \\ \mathbf{u}_v \end{bmatrix}.$$

Introducing

(56) $$\mathbf{E}_i = \mathbf{x}_{p,i0}^T\mathbf{x}_{p,i0}, \quad \mathbf{c}_{ui} = \mathbf{x}_{p,i0}^T\mathbf{x}_{u,i0}, \quad \mathbf{c}_{vi} = \mathbf{x}_{p,i0}^T\mathbf{x}_{v,i0},$$

(57) $$\gamma_{uui} = \mathbf{x}_{u,i0}^T\mathbf{x}_{u,i0}, \quad \gamma_{uvi} = \mathbf{x}_{u,i0}^T\mathbf{x}_{v,i0}, \quad \gamma_{vvi} = \mathbf{x}_{v,i0}^T\mathbf{x}_{v,i0},$$

(58) $$\varepsilon_{ui} = \mathbf{x}_{u,i0}^T\mathbf{x}_i', \quad \beta_{ui} = \mathbf{x}_{u,i0}^T\mathbf{x}_{i0}, \quad \beta_{vi} = \mathbf{x}_{v,i0}^T\mathbf{x}_{i0},$$

(59) $$\mathbf{b}_i = \mathbf{x}_{p,i0}^T\mathbf{x}_{i0}, \quad \mathbf{d}_i = \mathbf{x}_{p,i0}^T\mathbf{x}_i',$$

it is easy to show that

(60) $$\mathbf{N}_p = \mathbf{A}_p^T\mathbf{A}_p = \sum_{i=1}^{n}\mathbf{x}_{p,i0}^T\mathbf{x}_{p,i0} = \sum_{i=1}^{n}\mathbf{E}_i,$$

(61) $$\mathbf{N}_{pu} = \mathbf{A}_p^T\mathbf{A}_u = \left[\mathbf{x}_{p,10}^T\mathbf{x}_{u,10} \quad \cdots \quad \mathbf{x}_{p,n0}^T\mathbf{x}_{u,n0}\right] = \left[\mathbf{c}_{u1} \quad \cdots \quad \mathbf{c}_{un}\right],$$

(62) $$\mathbf{N}_{pv} = \mathbf{A}_p^T\mathbf{A}_v = \left[\mathbf{x}_{p,10}^T\mathbf{x}_{v,10} \quad \cdots \quad \mathbf{x}_{p,n0}^T\mathbf{x}_{v,n0}\right] = \left[\mathbf{c}_{v1} \quad \cdots \quad \mathbf{c}_{vn}\right],$$

(63) $$\mathbf{N}_u = \mathbf{A}_u^T\mathbf{A}_u = \begin{bmatrix} \mathbf{x}_{u,10}^T\mathbf{x}_{u,10} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \mathbf{x}_{u,n0}^T\mathbf{x}_{u,n0} \end{bmatrix} = \begin{bmatrix} \gamma_{uu1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \gamma_{uun} \end{bmatrix},$$

(64) $$\mathbf{N}_v = \mathbf{A}_v^T\mathbf{A}_v = \begin{bmatrix} \gamma_{vv1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \gamma_{vvn} \end{bmatrix}, \quad \mathbf{N}_{uv} = \mathbf{A}_u^T\mathbf{A}_v = \begin{bmatrix} \gamma_{uv1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \gamma_{uvn} \end{bmatrix},$$

(65) $$\mathbf{u}_p = \mathbf{A}_p^T\mathbf{b} = \sum_{i=1}^{n}\mathbf{x}_{p,i0}^T(\mathbf{x}_i' - \mathbf{x}_{i0}) = \sum_{i=1}^{n}(\mathbf{d}_i - \mathbf{b}_i),$$

(66) $$\mathbf{u}_u = \mathbf{A}_u^T\mathbf{b} = \begin{bmatrix} \mathbf{x}_{u,10}^T(\mathbf{x}_1' - \mathbf{x}_{10}) \\ \vdots \\ \mathbf{x}_{u,n0}^T(\mathbf{x}_n' - \mathbf{x}_{n0}) \end{bmatrix} = \begin{bmatrix} \varepsilon_{u1} - \beta_{u1} \\ \vdots \\ \varepsilon_{un} - \beta_{un} \end{bmatrix},$$

$$\mathbf{u}_v = \mathbf{A}_v^T\mathbf{b} = \begin{bmatrix} \mathbf{x}_{v,10}^T(\mathbf{x}_1' - \mathbf{x}_{10}) \\ \vdots \\ \mathbf{x}_{v,n0}^T(\mathbf{x}_n' - \mathbf{x}_{n0}) \end{bmatrix} = \begin{bmatrix} \varepsilon_{v1} - \beta_{v1} \\ \vdots \\ \varepsilon_{vn} - \beta_{vn} \end{bmatrix}.$$

Noting that the matrix $\begin{bmatrix} \mathbf{N}_u & \mathbf{N}_{uv} \\ \mathbf{N}_{uv}^T & \mathbf{N}_v \end{bmatrix}$ has all its submatrices diagonal, and recalling that multiplication of diagonal matrices is commutative, it is easy to verify that

$$\begin{bmatrix} \mathbf{N}_u & \mathbf{N}_{uv} \\ \mathbf{N}_{uv}^T & \mathbf{N}_v \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{\Delta}^{-1}\mathbf{N}_v & -\mathbf{\Delta}^{-1}\mathbf{N}_{uv} \\ -\mathbf{\Delta}^{-1}\mathbf{N}_{uv} & \mathbf{\Delta}^{-1}\mathbf{N}_u \end{bmatrix}, \tag{67}$$

where

$$\mathbf{\Delta} = \mathbf{N}_u\mathbf{N}_v - \mathbf{N}_{uv}^2 = \begin{bmatrix} \gamma_{uu1}\gamma_{vv1} - \gamma_{uv1}^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \gamma_{uun}\gamma_{vvn} - \gamma_{uvn}^2 \end{bmatrix} \equiv \begin{bmatrix} \delta_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \delta_n \end{bmatrix}, \tag{68}$$

$$\delta_i = \gamma_{uui}\gamma_{vvi} - \gamma_{uvi}^2 .$$

We will analytically invert

$$\begin{bmatrix} \begin{bmatrix} \mathbf{N}_p \end{bmatrix} & \begin{bmatrix} \mathbf{N}_{pu} & \mathbf{N}_{pv} \end{bmatrix} \\ \begin{bmatrix} \mathbf{N}_{pu}^T \\ \mathbf{N}_{pv}^T \end{bmatrix} & \begin{bmatrix} \mathbf{N}_u & \mathbf{N}_{uv} \\ \mathbf{N}_{uv}^T & \mathbf{N}_v \end{bmatrix} \end{bmatrix}^{-1} = \begin{bmatrix} \begin{bmatrix} \mathbf{Q}_p \end{bmatrix} & \begin{bmatrix} \mathbf{Q}_{pu} & \mathbf{Q}_{pv} \end{bmatrix} \\ \begin{bmatrix} \mathbf{Q}_{pu}^T \\ \mathbf{Q}_{pv}^T \end{bmatrix} & \begin{bmatrix} \mathbf{Q}_u & \mathbf{Q}_{uv} \\ \mathbf{Q}_{uv}^T & \mathbf{Q}_v \end{bmatrix} \end{bmatrix}, \tag{69}$$

using the well-known relations

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^T & \mathbf{D} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{X} & \mathbf{Y} \\ \mathbf{Y}^T & \mathbf{W} \end{bmatrix}, \qquad \mathbf{X} = (\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{B}^T)^{-1}, \tag{70}$$

$$\mathbf{Y} = -\mathbf{X}\mathbf{B}\mathbf{D}^{-1}, \qquad \mathbf{W} = \mathbf{D}^{-1} - \mathbf{D}^{-1}\mathbf{B}^T\mathbf{Y},$$

to obtain the recursive computation formulas

(71)
$$\mathbf{Q}_p = \left(\mathbf{N}_p - \mathbf{N}_{pu}\mathbf{\Delta}^{-1}\mathbf{N}_v\mathbf{N}_{pu}^T + \mathbf{N}_{pu}\mathbf{\Delta}^{-1}\mathbf{N}_{uv}\mathbf{N}_{pv}^T + \mathbf{N}_{pv}\mathbf{\Delta}^{-1}\mathbf{N}_{uv}\mathbf{N}_{pu}^T - \mathbf{N}_{pv}\mathbf{\Delta}^{-1}\mathbf{N}_u\mathbf{N}_{pv}^T\right)^{-1},$$

$$\mathbf{Q}_{pu} = \mathbf{Q}_p(-\mathbf{N}_{pu}\mathbf{\Delta}^{-1}\mathbf{N}_v + \mathbf{N}_{pv}\mathbf{\Delta}^{-1}\mathbf{N}_{uv}), \tag{72}$$

$$\mathbf{Q}_{pv} = \mathbf{Q}_p(\mathbf{N}_{pu}\mathbf{\Delta}^{-1}\mathbf{N}_{uv} - \mathbf{N}_{pv}\mathbf{\Delta}^{-1}\mathbf{N}_u), \tag{73}$$

$$\mathbf{Q}_u = \mathbf{\Delta}^{-1}\mathbf{N}_v + (-\mathbf{\Delta}^{-1}\mathbf{N}_v\mathbf{N}_{pu}^T + \mathbf{\Delta}^{-1}\mathbf{N}_{uv}\mathbf{N}_{pv}^T)\mathbf{Q}_{pu}, \tag{74}$$

$$\mathbf{Q}_{uv} = -\mathbf{\Delta}^{-1}\mathbf{N}_{uv} + (-\mathbf{\Delta}^{-1}\mathbf{N}_v\mathbf{N}_{pu}^T + \mathbf{\Delta}^{-1}\mathbf{N}_{uv}\mathbf{N}_{pv}^T)\mathbf{Q}_{pv}, \tag{75}$$

$$\mathbf{Q}_v = \mathbf{\Delta}^{-1}\mathbf{N}_u + (\mathbf{\Delta}^{-1}\mathbf{N}_{uv}\mathbf{N}_{pu}^T - \mathbf{\Delta}^{-1}\mathbf{N}_u\mathbf{N}_{pv}^T)\mathbf{Q}_{pv}. \tag{76}$$

With these submatrices the final solution can be calculated as

$$(77)\qquad \begin{bmatrix} \delta\hat{\mathbf{p}} \\ \delta\hat{\mathbf{u}} \\ \delta\hat{\mathbf{v}} \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_p & \mathbf{Q}_{pu} & \mathbf{Q}_{pv} \\ \mathbf{Q}_{pu}^T & \mathbf{Q}_u & \mathbf{Q}_{uv} \\ \mathbf{Q}_{pv}^T & \mathbf{Q}_{uv}^T & \mathbf{Q}_v \end{bmatrix} \begin{bmatrix} \mathbf{u}_p \\ \mathbf{u}_u \\ \mathbf{u}_v \end{bmatrix}.$$

The obtained estimates $\hat{\mathbf{p}} = \mathbf{p}_0 + \delta\hat{\mathbf{p}}$, $\hat{\mathbf{u}} = \mathbf{u}_0 + \delta\hat{\mathbf{u}}$, $\hat{\mathbf{v}} = \mathbf{v}_0 + \delta\hat{\mathbf{v}}$ are used as approximate values in the next iteration step and so on until convergence is achieved. One can also use any appropriate algorithm to project the points $\mathbf{x}_i'$ on the ellipsoid with parameters $\hat{\mathbf{p}} = \mathbf{p}_0 + \delta\hat{\mathbf{p}}$ (see e.g. the proposed approach in appendix A) to obtain estimates $\hat{u}_i$, $\hat{v}_i$, which together with $\hat{\mathbf{p}}$ will serve as approximate values for the next iteration step. Thus only $\delta\hat{\mathbf{p}} = \mathbf{Q}_p\mathbf{u}_p + \mathbf{Q}_{pu}\mathbf{u}_u + \mathbf{Q}_{pv}\mathbf{u}_v$ needs to be used.

## 7. Application to the case of the triaxial ellipsoid

<u>Implicit representation – Nonlinear normal equations</u>

With the values of $f(\mathbf{x},\mathbf{a},\mathbf{b})$, $\mathbf{g}$, and $\mathbf{z}$, derived in appendix A for the case of the triaxial ellipsoid, the nonlinear normal equations (20)-(22) take the specific form

$$(78)\qquad \mathbf{x}_i' - \hat{\mathbf{x}}_i + \hat{\lambda}_i(2\hat{\mathbf{A}}\hat{\mathbf{x}}_i + \hat{\mathbf{b}}) = \mathbf{x}_i' - \hat{\mathbf{x}}_i + \hat{\lambda}_i[2\mathbf{Q}(\hat{\mathbf{x}}_i)^T\hat{\mathbf{a}} + \hat{\mathbf{b}}] = \mathbf{0}, \qquad i = 1,2,\ldots,n.$$

$$(79)\qquad \sum_{i=1}^{n} \hat{\lambda}_i \mathbf{q}(\hat{\mathbf{x}}_i) = \mathbf{0},$$

$$(80)\qquad \sum_{i=1}^{n} \hat{\lambda}_i \hat{\mathbf{x}}_i = \mathbf{0},$$

$$(81)\qquad \hat{\mathbf{x}}_i^T\hat{\mathbf{A}}\hat{\mathbf{x}}_i + \hat{\mathbf{b}}^T\hat{\mathbf{x}}_i + 1 = \mathbf{q}(\hat{\mathbf{x}}_i)^T\hat{\mathbf{a}} + \hat{\mathbf{b}}^T\hat{\mathbf{x}}_i + 1 = 0, \qquad i = 1,2,\ldots,n.$$

with $\mathbf{q}(\mathbf{x})$ and $\mathbf{Q}(\mathbf{x})$ as defined in appendix A, equation (A15). The solution is obtained by using any of the standard methods for solving systems of nonlinear equations, which typically implement an iteration process.

<u>Implicit representation – Linearization</u>

With the values derived in appendix A we have

$$(82)\qquad f_{0i} = f(\mathbf{x}_{i0},\mathbf{p}_0) = \mathbf{x}_{i0}^T\mathbf{A}_0\mathbf{x}_{i0} + \mathbf{b}_0^T\mathbf{x}_{i0} + 1 = \mathbf{q}(\mathbf{x}_{i0})^T\mathbf{a}_0 + \mathbf{b}_0^T\mathbf{x}_{i0} + 1$$

$$(83)\qquad \mathbf{g}_{i0} = (2\mathbf{A}_0\mathbf{x}_{i0} + \mathbf{b}_0) = 2\mathbf{Q}(\mathbf{x}_{i0})^T\mathbf{a}_0 + \mathbf{b}_0,$$

$$(84)\qquad \mathbf{z}_{0i} = \begin{bmatrix} \mathbf{q}(\mathbf{x}_{0i})^T & \mathbf{x}_{0i}^T \end{bmatrix}^T = \begin{bmatrix} \mathbf{q}(\mathbf{x}_{0i}) \\ \mathbf{x}_{0i} \end{bmatrix},$$

(85) $\kappa_{i0} = (2\mathbf{A}_0\mathbf{x}_{i0} + \mathbf{b}_0)^T(2\mathbf{A}_0\mathbf{x}_{i0} + \mathbf{b}_0) = [2\mathbf{Q}(\mathbf{x}_{i0})^T\mathbf{a}_0 + \mathbf{b}_0]^T[2\mathbf{Q}(\mathbf{x}_{i0})^T\mathbf{a}_0 + \mathbf{b}_0]$,

and the solution (36), (37) takes the explicit form

(86)
$$\delta\hat{\mathbf{p}} = \begin{bmatrix} \delta\hat{\mathbf{a}} \\ \delta\hat{\mathbf{b}} \end{bmatrix} = -\begin{bmatrix} \sum_{i=1}^{n} \frac{1}{\kappa_{i0}}\mathbf{q}(\mathbf{x}_{i0})\mathbf{q}(\mathbf{x}_{i0})^T & \sum_{i=1}^{n} \frac{1}{\kappa_{i0}}\mathbf{q}(\mathbf{x}_{i0})\mathbf{x}_{0i}^T \\ \sum_{i=1}^{n} \frac{1}{\kappa_{i0}}\mathbf{x}_{0i}\mathbf{q}(\mathbf{x}_{i0})^T & \sum_{i=1}^{n} \frac{1}{\kappa_{i0}}\mathbf{x}_{0i}\mathbf{x}_{0i}^T \end{bmatrix}^{-1} \cdot \begin{bmatrix} \sum_{i=1}^{n} \frac{(2\mathbf{A}_0\mathbf{x}_{i0} + \mathbf{b}_0)^T(\mathbf{x}'_i - \mathbf{x}_{i0}) + f_{i0}}{\kappa_{i0}}\mathbf{q}(\mathbf{x}_{i0}) \\ \sum_{i=1}^{n} \frac{(2\mathbf{A}_0\mathbf{x}_{i0} + \mathbf{b}_0)^T(\mathbf{x}'_i - \mathbf{x}_{i0}) + f_{i0}}{\kappa_{i0}}\mathbf{x}_{0i} \end{bmatrix},$$

(87)
$$\delta\hat{\mathbf{x}}_i = \mathbf{x}'_i - \mathbf{x}_{i0} - \frac{(2\mathbf{A}_0\mathbf{x}_{i0} + \mathbf{b}_0)^T(\mathbf{x}'_i - \mathbf{x}_{i0}) + f_{i0}}{\kappa_{i0}}(2\mathbf{A}_0\mathbf{x}_{i0} + \mathbf{b}_0) - \\ - \frac{1}{\kappa_{i0}}(2\mathbf{A}_0\mathbf{x}_{i0} + \mathbf{b}_0)\left[\mathbf{q}(\mathbf{x}_{i0})^T\delta\hat{\mathbf{a}} + \mathbf{x}_{0i}^T\delta\hat{\mathbf{b}}\right], \quad i = 1, 2, \ldots, n.$$

It is also possible to use only equation (86) to compute $\delta\hat{\mathbf{p}}$ and $\hat{\mathbf{p}} = \mathbf{p}_0 + \delta\hat{\mathbf{p}}$. Estimates $\hat{\mathbf{x}}_i$ can be obtained by projecting each $\mathbf{x}'_i$ on the ellipsoid defined by $\hat{\mathbf{p}}$ using any projection algorithm (see e.g. the proposed approach in appendix A).

Parametric representation – Nonlinear normal equations

In order to derive the nonlinear normal equations of the form (48)-(50) we just need to compute the relevant functions, utilizing the results from appendix A. With $\mathbf{x} = \mathbf{R}^T(\overline{\mathbf{x}} + \overline{\mathbf{d}})$, $\mathbf{x}_u = \mathbf{R}^T\overline{\mathbf{x}}_u$, $\mathbf{x}_v = \mathbf{R}^T\overline{\mathbf{x}}_v$ we obtain

(88) $\beta_u = \overline{\mathbf{x}}^T\overline{\mathbf{x}}_u + \overline{\mathbf{d}}^T\overline{\mathbf{x}}_u = (a_Y^2 - a_X^2)\cos u \sin u \sin^2 v + (-\overline{d}_X a_X \sin u + \overline{d}_Y a_Y \cos u)\sin v$,

(89)
$$\beta_v = \overline{\mathbf{x}}^T\overline{\mathbf{x}}_v + \overline{\mathbf{d}}^T\overline{\mathbf{x}}_v = \\ = (a_X^2\cos^2 u + a_Y^2\sin^2 u - a_Z^2)\sin v\cos v + (\overline{d}_X a_X \cos u + \overline{d}_Y a_Y \sin u)\cos v - \overline{d}_Z a_Z \sin v,$$

(90)
$$\varepsilon_u = \mathbf{x}'^T\mathbf{R}^T\overline{\mathbf{x}}_u, \qquad \varepsilon_v = \mathbf{x}'^T\mathbf{R}^T\overline{\mathbf{x}}_v,$$

(91)
$$\mathbf{b}_p = \mathbf{x}_p^T\mathbf{x} = \mathbf{x}_p^T\mathbf{R}^T(\overline{\mathbf{x}} + \overline{\mathbf{d}}) = \begin{bmatrix} \mathbf{0} \\ \overline{\mathbf{x}} + \overline{\mathbf{d}} \\ \mathbf{D}(\overline{\mathbf{x}} + \overline{\mathbf{d}}) \end{bmatrix}, \quad \mathbf{e}_p = \mathbf{x}_p^T\mathbf{x}' = \begin{bmatrix} -\mathbf{\Omega}^T[(\overline{\mathbf{x}} + \overline{\mathbf{d}})\times]\mathbf{R}\mathbf{x}' \\ \mathbf{R}\mathbf{x}' \\ \mathbf{D}\mathbf{R}\mathbf{x}' \end{bmatrix}.$$

With the above values, equation (48) splits into three equations

$$\mathbf{\Omega}(\boldsymbol{\theta})^T \sum_{i=1}^{n} [\{\overline{\mathbf{x}}(\boldsymbol{\alpha}, u_i, v_i) + \overline{\mathbf{d}}\}\times]\mathbf{R}(\boldsymbol{\theta})\mathbf{x}_i' = \mathbf{0}, \tag{92}$$

$$\mathbf{R}(\boldsymbol{\theta})\sum_{i=1}^{n} \mathbf{x}_i' - \sum_{i=1}^{n} \overline{\mathbf{x}}(\boldsymbol{\alpha}, u_i, v_i) - n\overline{\mathbf{d}} = \mathbf{0}, \tag{93}$$

$$\sum_{i=1}^{n} \mathbf{D}(u_i, v_i)\left[\mathbf{R}(\boldsymbol{\theta})\mathbf{x}_i' - \overline{\mathbf{x}}(\boldsymbol{\alpha}, u_i, v_i) - \overline{\mathbf{d}}\right] = \mathbf{0}, \tag{94}$$

where the factor $\mathbf{\Omega}(\boldsymbol{\theta})^T$ in (92) can be deleted due to the fact that in general $\det \mathbf{\Omega} = -\cos\theta_2 \cos 2\theta_3 \neq 0$.

Equations (49) and (50) become

$$\mathbf{x}_i'^T \mathbf{R}(\boldsymbol{\theta})^T \overline{\mathbf{x}}_u(\boldsymbol{\alpha}, u_i, v_i) - \beta_u(\boldsymbol{\alpha}, \overline{\mathbf{d}}, u_i, v_i) = 0, \qquad i = 1, 2, ..., n, \tag{95}$$

$$\mathbf{x}_i'^T \mathbf{R}(\boldsymbol{\theta})^T \overline{\mathbf{x}}_v(\boldsymbol{\alpha}, u_i, v_i) - \beta_v(\boldsymbol{\alpha}, \overline{\mathbf{d}}, u_i, v_i) = 0, \qquad i = 1, 2, ..., n. \tag{96}$$

Again, (92)-(96) is a system of $3+3+3+2n = 9+2n$ nonlinear equations in $9+2n$ unknowns $\boldsymbol{\theta}$, $\boldsymbol{\alpha}$, $\overline{\mathbf{d}}$ and $\{u_i, v_i\}$, $i = 1,...,n$, to be solved by one of the various existing methods.

Parametric representation – Linearization

In order to apply the general solution (60)-(66) and (71)-(77), we must use the results of appendix A and evaluate the necessary functions for approximate values $u_{i0}$, $v_{i0}$, $a_{X0}$, $a_{Y0}$, $a_{Z0}$, $\boldsymbol{\theta}_0$, $\overline{\mathbf{d}}_0$. With $\mathbf{R}_0 = \mathbf{R}(\boldsymbol{\theta}_0)$ and $\mathbf{\Omega}_0 = \mathbf{\Omega}(\boldsymbol{\theta}_0)$ and setting

$$\overline{\mathbf{x}}_{i0}' = \mathbf{R}_0 \mathbf{x}_i', \qquad \mathbf{D}_{i0} = \mathbf{D}(u_{i0}, v_{i0}), \tag{97}$$

we have

$$\mathbf{E}_i = \mathbf{x}_{p,i0}\mathbf{x}_{p,i0}^T = \begin{bmatrix} -\mathbf{\Omega}_0^T[(\overline{\mathbf{x}}_{i0} + \overline{\mathbf{d}}_0)\times]^2\mathbf{\Omega}_0 & -\mathbf{\Omega}_0^T[(\overline{\mathbf{x}}_{i0} + \overline{\mathbf{d}}_0)\times] & -\mathbf{\Omega}_0^T[(\overline{\mathbf{x}}_{i0} + \overline{\mathbf{d}}_0)\times]\mathbf{D} \\ [(\overline{\mathbf{x}}_{i0} + \overline{\mathbf{d}}_0)\times]\mathbf{\Omega}_0 & \mathbf{I} & \mathbf{D}_{i0} \\ \mathbf{D}_{i0}[(\overline{\mathbf{x}}_{i0} + \overline{\mathbf{d}}_0)\times]\mathbf{\Omega}_0 & \mathbf{D}_{i0} & \mathbf{D}_{i0}^2 \end{bmatrix}, \tag{98}$$

$$\mathbf{c}_{ui} = \begin{bmatrix} \mathbf{\Omega}_0^T[\overline{\mathbf{x}}_{u,i0}\times](\overline{\mathbf{x}}_{i0} + \overline{\mathbf{d}}_0) \\ \overline{\mathbf{x}}_{u,i0} \\ \mathbf{D}_{i0}\overline{\mathbf{x}}_{u,i0} \end{bmatrix}, \qquad \mathbf{c}_{vi} = \begin{bmatrix} \mathbf{\Omega}_0^T[\overline{\mathbf{x}}_{v,i0}\times](\overline{\mathbf{x}}_{i0} + \overline{\mathbf{d}}_0) \\ \overline{\mathbf{x}}_{v,i0} \\ \mathbf{D}_{i0}\overline{\mathbf{x}}_{v,i0} \end{bmatrix}, \tag{99}$$

$$\gamma_{uui} = (a_{X0}^2 \sin^2 u_{i0} + a_{Y0}^2 \cos^2 u_{i0})\sin^2 v_{i0}, \tag{100}$$

$$\gamma_{uvi} = (a_{Y0}^2 - a_{X0}^2)\sin u_{i0} \cos u_{i0} \sin v_{i0} \cos v_{i0}, \tag{101}$$

$$\gamma_{vvi} = (a_{X0}^2 \cos^2 u_{i0} + a_{Y0}^2 \sin^2 u_{i0})\cos^2 v_{i0} + a_{Z0}^2 \sin^2 v_{i0}, \tag{102}$$

(103) $$\varepsilon_{ui} = \overline{\mathbf{x}}_{i0}'^{\mathrm{T}} \overline{\mathbf{x}}_{u,i0}, \quad \varepsilon_{vi} = \overline{\mathbf{x}}_{i0}'^{T} \overline{\mathbf{x}}_{v,i0},$$

(104) $$\beta_{ui} = (a_{Y0}^2 - a_{X0}^2)\cos u_{i0} \sin u_{i0} \sin^2 v_{i0} + (-\overline{d}_{X0} a_{X0} \sin u_{i0} + \overline{d}_{Y0} a_{Y0} \cos u_{i0}) \sin v_{i0}$$

(105) $$\beta_{vi} = (a_{X0}^2 \cos^2 u_{i0} + a_{Y0}^2 \sin^2 u_{i0} - a_{Z0}^2) \sin v_{i0} \cos v_{i0} + \\ +(\overline{d}_{X0} a_{X0} \cos u_{i0} + \overline{d}_{Y0} a_{Y0} \sin u_{i0}) \cos v_{i0} - \overline{d}_{Z0} a_{Z0} \sin v_{i0}$$

(106) $$\mathbf{b}_i = \begin{bmatrix} \mathbf{0} \\ \overline{\mathbf{x}}_{i0} + \overline{\mathbf{d}}_0 \\ \mathbf{D}_{i0}^T (\overline{\mathbf{x}}_{i0} + \overline{\mathbf{d}}_0) \end{bmatrix}, \quad \mathbf{d}_i = \begin{bmatrix} -\mathbf{\Omega}_0^T [(\overline{\mathbf{x}}_{0i} + \overline{\mathbf{d}}_0) \times] \overline{\mathbf{x}}_{0i}' \\ \overline{\mathbf{x}}_{0i}' \\ \mathbf{D}_{0i} \overline{\mathbf{x}}_{0i}' \end{bmatrix}.$$

With the above values we can directly formulate all the necessary submatrices of the normal equations (60)-(66) and (71)-(76), in order to calculate the solution (77), or just the solution for $\delta\hat{\mathbf{p}}$, completed by projections of the $\mathbf{x}_i'$ on the surface of the resulting ellipsoid to obtain the $\hat{\mathbf{x}}_i$ estimates.

<u>Initial approximate values using the algebraic approach</u>

In any iterative solution approach it is essential to have good initial approximate values so that convergence can be achieved. Such desired values can be provided by the algebraic approach where one minimizes instead

(107) $$\phi = \sum_{i=1}^{n} f(\mathbf{x}_i', \mathbf{p})^2 = \min .$$

Setting the derivatives of the above target function with respect to the single parameters $\mathbf{p}$ we obtain

(108) $$\frac{\partial \phi}{\partial \mathbf{p}} = 2\sum_{i=1}^{n} f(\mathbf{x}_i', \mathbf{p}) \frac{\partial f}{\partial \mathbf{p}}(\mathbf{x}_i', \mathbf{p}) = \sum_{i=1}^{n} f(\mathbf{x}_i', \mathbf{p}) \mathbf{z}^T(\mathbf{x}_i', \mathbf{p}) = \mathbf{0},$$

and the nonlinear normal equations for the algebraic approach become

(109) $$\sum_{i=1}^{n} \mathbf{z}(\mathbf{x}_i', \hat{\mathbf{p}}) f(\mathbf{x}_i', \hat{\mathbf{p}}) = \mathbf{0}.$$

For application to the case of the ellipsoid we need to replace

(110) $$\mathbf{z}(\mathbf{x}_i', \hat{\mathbf{p}}) = \begin{bmatrix} \mathbf{q}(\mathbf{x}_i') \\ \mathbf{x}_i' \end{bmatrix}, \quad f(\mathbf{x}_i', \hat{\mathbf{p}}) = \mathbf{q}(\mathbf{x}_i')^T \hat{\mathbf{a}} + \mathbf{x}_i'^T \hat{\mathbf{b}} + 1$$

to obtain

(111) $$\sum_{i=1}^{n} \begin{bmatrix} \mathbf{q}(\mathbf{x}_i') \\ \mathbf{x}_i' \end{bmatrix} \left[ \mathbf{q}(\mathbf{x}_i')^T \hat{\mathbf{a}} + \mathbf{x}_i'^T \hat{\mathbf{b}} + 1 \right] = \mathbf{0}.$$

This is a linear system in the unknowns $\hat{\mathbf{p}} = \begin{bmatrix} \hat{\mathbf{a}} \\ \hat{\mathbf{b}} \end{bmatrix}$ and has solution

$$(112) \qquad \begin{bmatrix} \hat{\mathbf{a}} \\ \hat{\mathbf{b}} \end{bmatrix} = -\begin{bmatrix} \sum_{i=1}^{n} \mathbf{q}(\mathbf{x}_i')\mathbf{q}(\mathbf{x}_i')^T & \sum_{i=1}^{n} \mathbf{q}(\mathbf{x}_i')\mathbf{x}_i'^T \\ \sum_{i=1}^{n} \mathbf{x}_i'\mathbf{q}(\mathbf{x}_i')^T & \sum_{i=1}^{n} \mathbf{x}_i'\mathbf{x}_i'^T \end{bmatrix}^{-1} \begin{bmatrix} \sum_{i=1}^{n} \mathbf{q}(\mathbf{x}_i') \\ \sum_{i=1}^{n} \mathbf{x}_i' \end{bmatrix}$$

where

$$(113) \qquad \mathbf{x}_i' = \begin{bmatrix} X_i' \\ Y_i' \\ Z_i' \end{bmatrix}, \quad \mathbf{q}(\mathbf{x}_i') = \begin{bmatrix} X_i'^2 & 2X_i'Y_i' & 2X_i'Z_i' & Y_i'^2 & 2Y_i'Z_i' & Z_i'^2 \end{bmatrix}^T .$$

## Appendix A: Analytical representation of the triaxial ellipsoid

The implicit representation

Let $\bar{\mathbf{x}} = [\bar{X}\ \bar{Y}\ \bar{Z}]^T$ be the coordinates of any point on the surface of a triaxial ellipsoid with respect to a reference system with origin at the ellipsoid center and axes along the ellipsoid axes. The well-known equation of the triaxial ellipsoid is

$$\text{(A1)}\qquad 1 = \frac{\bar{X}^2}{\alpha_X^2} + \frac{\bar{Y}^2}{\alpha_Y^2} + \frac{\bar{Z}^2}{\alpha_Z^2} = \begin{bmatrix} \bar{X} & \bar{Y} & \bar{Z} \end{bmatrix} \begin{bmatrix} \alpha_X^{-2} & 0 & 0 \\ 0 & \alpha_Y^{-2} & 0 \\ 0 & 0 & \alpha_Z^{-2} \end{bmatrix} \begin{bmatrix} \bar{X} \\ \bar{Y} \\ \bar{Z} \end{bmatrix} \equiv \bar{\mathbf{x}}^T \mathbf{\Lambda} \bar{\mathbf{x}} = 1 ,$$

where $\alpha_X$, $\alpha_Y$, $\alpha_Z$ are the ellipsoid semi-axes. If $\mathbf{x} = [X\,Y\,Z]^T$ are the coordinates of the same point in an arbitrary reference system then it holds that

$$\text{(A2)}\qquad \bar{\mathbf{x}} = \mathbf{R}(\mathbf{x} - \mathbf{d}) , \quad \mathbf{x} = \mathbf{R}^T \bar{\mathbf{x}} + \mathbf{d} = \mathbf{R}^T (\bar{\mathbf{x}} + \bar{\mathbf{d}}) , \quad (\bar{\mathbf{d}} = \mathbf{R}\mathbf{d}),$$

where $\mathbf{d} = [d_X\ d_Y\ d_Z]^T$ are the coordinates of the ellipsoid center in the arbitrary reference system and $\mathbf{R}$ an orthogonal rotation matrix. Therefore, the ellipsoid equation in the arbitrary reference system becomes

$$\text{(A3)}\qquad 1 = (\mathbf{x} - \mathbf{d})^T \mathbf{R}^T \mathbf{\Lambda} \mathbf{R} (\mathbf{x} - \mathbf{d}) = \mathbf{x}^T \mathbf{R}^T \mathbf{\Lambda} \mathbf{R} \mathbf{x} - 2 \mathbf{d}^T \mathbf{R}^T \Lambda \mathbf{R} \mathbf{x} + \mathbf{d}^T \mathbf{R}^T \mathbf{\Lambda} \mathbf{R} \mathbf{d} = 1 ,$$

or

$$\text{(A4)}\qquad \mathbf{x}^T \left( \frac{1}{\mathbf{d}^T \mathbf{R}^T \mathbf{\Lambda} \mathbf{R} \mathbf{d} - 1} \mathbf{R}^T \mathbf{\Lambda} \mathbf{R} \right) \mathbf{x} - \left( \frac{2}{\mathbf{d}^T \mathbf{R}^T \mathbf{\Lambda} \mathbf{R} \mathbf{d} - 1} \mathbf{R}^T \mathbf{\Lambda} \mathbf{R} \mathbf{d} \right)^T \mathbf{x} + 1 =$$

$$= \mathbf{x}^T \mathbf{A} \mathbf{x} + \mathbf{b}^T \mathbf{x} + 1 = 0 ,$$

where

$$\text{(A5)}\qquad \mathbf{A} = \frac{1}{\mathbf{d}^T \mathbf{R}^T \mathbf{\Lambda} \mathbf{R} \mathbf{d} - 1} \mathbf{R}^T \mathbf{\Lambda} \mathbf{R} = \mathbf{A}^T , \quad \mathbf{b} = -\frac{2}{\mathbf{d}^T \mathbf{R}^T \mathbf{\Lambda} \mathbf{R} \mathbf{d} - 1} \mathbf{R}^T \mathbf{\Lambda} \mathbf{R} \mathbf{d} .$$

Here we have “normalized” equation (A3) by dividing with $\mathbf{d}^T \mathbf{R}^T \mathbf{\Lambda} \mathbf{R} \mathbf{d} - 1$ to make the constant term equal to 1. For alternative normalizations see Turner, Anderson, Mason & Cox (1999).

We have now a simple algebraic representation in terms of the nine ellipsoid parameters

$$\text{(A6)}\qquad \mathbf{a} = [A_{11}\ A_{12}\ A_{13}\ A_{22}\ A_{23}\ A_{33}]^T , \quad \mathbf{b} = [b_1\ b_2\ b_3]^T .$$

If these parameters are determined one should like to convert them to the parameters, $a_X$, $a_Y$, $a_Z$, $d_X$, $d_Y$, $d_Z$ and three parameters defining the rotation matrix $\mathbf{R}$. To solve this inversion problem we may use a standard diagonalization algorithm to obtain

(A7) $$\mathbf{A} = \mathbf{R}^T \mathbf{M} \mathbf{R},$$

which gives directly the required matrix $\mathbf{R}$, and the diagonal matrix $\mathbf{M}$ satisfying

(A8) $$\mathbf{M} = \frac{1}{\mathbf{d}^T \mathbf{R}^T \boldsymbol{\Lambda} \mathbf{R} \mathbf{d} - 1} \boldsymbol{\Lambda}, \Rightarrow \quad -2\mathbf{R}^T \mathbf{M} \mathbf{R} \mathbf{d} = -\frac{2}{\mathbf{d}^T \mathbf{R}^T \boldsymbol{\Lambda} \mathbf{R} \mathbf{d} - 1} \mathbf{R}^T \boldsymbol{\Lambda} \mathbf{R} \mathbf{d} = \mathbf{b}.$$

Solving the last equation for $\mathbf{d}$ we obtain

(A9) $$\mathbf{d} = -\frac{1}{2} \mathbf{R}^T \mathbf{M}^{-1} \mathbf{R} \mathbf{b}.$$

It remains to solve $\mathbf{M} = \frac{1}{\mathbf{d}^T \mathbf{R}^T \boldsymbol{\Lambda} \mathbf{R} \mathbf{d} - 1} \boldsymbol{\Lambda}$ for $\boldsymbol{\Lambda}$, which contains the semiaxes $a_X$, $a_Y$, $a_Z$. Setting $\mathbf{q} = \mathbf{R}\mathbf{d} = -\frac{1}{2} \mathbf{M}^{-1} \mathbf{R} \mathbf{b}$ the equation to solve becomes $\mathbf{M} = \frac{1}{\mathbf{q}^T \boldsymbol{\Lambda} \mathbf{q} - 1} \boldsymbol{\Lambda}$, with corresponding diagonal elements satisfying

(A10) $$M_{ii} = \frac{1}{q_1^2 \Lambda_{11} + q_2^2 \Lambda_{22} + q_3^2 \Lambda_{33} - 1} \Lambda_{ii},$$

$$(q_1^2 \Lambda_{11} + q_2^2 \Lambda_{22} + q_3^2 \Lambda_{33}) M_{ii} + \Lambda_{ii} = M_{ii}, \qquad 1 = 1,2,3.$$

The solution of the last system is

(A11) $$\begin{bmatrix} \Lambda_{11} \\ \Lambda_{22} \\ \Lambda_{33} \end{bmatrix} = \begin{bmatrix} M_{11} q_1^2 - 1 & M_{11} q_2^2 & M_{11} q_3^2 \\ M_{22} q_1^2 & M_{22} q_2^2 - 1 & M_{22} q_3^2 \\ M_{33} q_1^2 & M_{33} q_2^2 & M_{33} q_3^2 - 1 \end{bmatrix}^{-1} \begin{bmatrix} M_{11} \\ M_{22} \\ M_{33} \end{bmatrix}.$$

Thus the transformation of $\mathbf{A}$ and $\mathbf{b}$ into $\mathbf{R}$, $\mathbf{d}$ and $\boldsymbol{\Lambda}$ ($\alpha_X, \alpha_Y, \alpha_Z$) has been completed.

The algebraic representation has also the alternative form

(A12) $$f(\mathbf{x}, \mathbf{a}, \mathbf{b}) = \mathbf{x}^T \mathbf{A} \mathbf{x} + \mathbf{b}^T \mathbf{x} + 1 = \mathbf{q}(\mathbf{x})^T \mathbf{a} + \mathbf{b}^T \mathbf{x} + 1 = 0.$$

This results from the fact that

(A13) $$\mathbf{A}\mathbf{x} = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{12} & A_{22} & A_{23} \\ A_{13} & A_{23} & A_{33} \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} = \begin{bmatrix} A_{11} X + A_{12} Y + A_{13} Z \\ A_{12} X + A_{22} Y + A_{23} Z \\ A_{13} X + A_{23} Y + A_{33} Z \end{bmatrix} =$$

$$
= \begin{bmatrix} X & Y & Z & 0 & 0 & 0 \\ 0 & X & 0 & Y & Z & 0 \\ 0 & 0 & X & 0 & Y & Z \end{bmatrix} \begin{bmatrix} A_{11} \\ A_{12} \\ A_{13} \\ A_{22} \\ A_{23} \\ A_{33} \end{bmatrix} \equiv \mathbf{Q}(\mathbf{x})^T \mathbf{a} ,
$$

and

(A14) $$\mathbf{x}^T \mathbf{A}\mathbf{x} = \mathbf{x}^T \mathbf{Q}(\mathbf{x})^T \mathbf{a} \equiv \mathbf{q}(\mathbf{x})^T \mathbf{a} ,$$

where

(A15) $$\mathbf{Q}(\mathbf{x}) = \begin{bmatrix} X & 0 & 0 \\ Y & X & 0 \\ Z & 0 & X \\ 0 & Y & 0 \\ 0 & Z & Y \\ 0 & 0 & Z \end{bmatrix}, \quad \mathbf{q}(\mathbf{x}) = \mathbf{Q}(\mathbf{x})\mathbf{x} = \begin{bmatrix} X & 0 & 0 \\ Y & X & 0 \\ Z & 0 & X \\ 0 & Y & 0 \\ 0 & Z & Y \\ 0 & 0 & Z \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} = \begin{bmatrix} X^2 \\ 2XY \\ 2XZ \\ Y^2 \\ 2YZ \\ Z^2 \end{bmatrix} .$$

We need also to compute the following derivatives

(A16) $$\mathbf{g} = \left( \frac{\partial f}{\partial \mathbf{x}} \right)^T = 2\mathbf{A}\mathbf{x} + \mathbf{b} = 2\mathbf{Q}(\mathbf{x})^T \mathbf{a} + \mathbf{b} ,$$

(A17) $$\mathbf{z} = \left( \frac{\partial f}{\partial \mathbf{p}} \right)^T = \begin{bmatrix} \frac{\partial f}{\partial \mathbf{a}} & \frac{\partial f}{\partial \mathbf{b}} \end{bmatrix}^T = \begin{bmatrix} \mathbf{q}(\mathbf{x})^T & \mathbf{x}^T \end{bmatrix}^T = \begin{bmatrix} \mathbf{q}(\mathbf{x}) \\ \mathbf{x} \end{bmatrix} .$$

<u>The parametric representation</u>

Among various parametric representations of the triaxial ellipsoid the one more convenient for our purpose has the following form in the reference system $\bar{\mathbf{x}} = \mathbf{R}(\mathbf{x} - \mathbf{d})$ attached to the ellipsoid center and axes

(A18) $$\bar{\mathbf{x}} = \begin{bmatrix} \bar{X} \\ \bar{Y} \\ \bar{Z} \end{bmatrix} = \begin{bmatrix} \alpha_X \cos u \sin v \\ \alpha_Y \sin u \sin v \\ \alpha_Z \cos v \end{bmatrix} = \bar{\mathbf{x}}(\alpha_X, \alpha_Y, \alpha_Z, u, v) .$$

This form follows by rewriting the implicit representation as $(\bar{X}/\alpha_X)^2 + (\bar{Y}/\alpha_Y)^2 + (\bar{Z}/\alpha_Z)^2 = 1$ and thus realizing that $\bar{X}/\alpha_X$, $\bar{Y}/\alpha_Y$, $\bar{Z}/\alpha_Z$ are the components of a unit vector $\bar{\mathbf{n}}$ which can be expressed in terms of its longitude $u$ ($0 \le u < 2\pi$) and its co-latitude $v$ ($0 \le v \le \pi$) as

$\bar{\mathbf{n}} = \left[\cos u \sin v \quad \sin u \sin v \quad \cos v\right]^T$. In the arbitrary reference system the representation becomes

(A19) $$\mathbf{x} = \mathbf{R}(\boldsymbol{\theta})^T [\bar{\mathbf{x}}(\boldsymbol{\alpha}, u, v) + \bar{\mathbf{d}}] = \mathbf{x}(\mathbf{p}, u, v),$$

where $\mathbf{p} = [\theta_1\, \theta_2\, \theta_3\; \bar{d}_X\, \bar{d}_Y\, \bar{d}_Z\; \alpha_X\, \alpha_Y\, \alpha_Z]^T$, $\boldsymbol{\alpha} = [\alpha_X\, \alpha_Y\, \alpha_Z]^T$, $\bar{\mathbf{d}} = [\bar{d}_X\, \bar{d}_Y\, \bar{d}_Z]^T$ and $\boldsymbol{\theta} = [\theta_1\, \theta_2\, \theta_3]^T$ are the rotation angles around the three axes, which define the rotation matrix $\mathbf{R}(\boldsymbol{\theta}) = \mathbf{R}_3(\theta_3)\mathbf{R}_2(\theta_2)\mathbf{R}_1(\theta_1)$.
We will need the derivatives

(A20) $$\bar{\mathbf{x}}_u \equiv \frac{\partial \bar{\mathbf{x}}}{\partial u} = \begin{bmatrix} -\alpha_X \sin u \sin v \\ \alpha_Y \cos u \sin v \\ 0 \end{bmatrix}, \quad \bar{\mathbf{x}}_v \equiv \frac{\partial \bar{\mathbf{x}}}{\partial v} = \begin{bmatrix} \alpha_X \cos u \cos v \\ \alpha_Y \sin u \cos v \\ -\alpha_Z \sin v \end{bmatrix},$$

(A21) $$\mathbf{x}_u \equiv \frac{\partial \mathbf{x}}{\partial u} = \mathbf{R}(\boldsymbol{\theta})^T \bar{\mathbf{x}}_u, \quad \mathbf{x}_v \equiv \frac{\partial \mathbf{x}}{\partial v} = \mathbf{R}(\boldsymbol{\theta})^T \bar{\mathbf{x}}_v.$$

Setting

(A22) $$[\boldsymbol{\omega}_k \times] = \frac{\partial \mathbf{R}}{\partial \theta_k} \mathbf{R}^T, \quad \boldsymbol{\Omega} = [\boldsymbol{\omega}_1\, \boldsymbol{\omega}_2\, \boldsymbol{\omega}_3],$$

we have $\dfrac{\partial \mathbf{R}^T}{\partial \theta_k} = -\mathbf{R}^T [\boldsymbol{\omega}_k \times]$ and for any vector $\mathbf{q}$

(A23) $$\frac{\partial(\mathbf{R}^T \mathbf{q})}{\partial \boldsymbol{\theta}} = \left[ \frac{\partial \mathbf{R}^T}{\partial \theta_1}\mathbf{q} \quad \frac{\partial \mathbf{R}^T}{\partial \theta_1}\mathbf{q} \quad \frac{\partial \mathbf{R}^T}{\partial \theta_1}\mathbf{q} \right] =$$
$$= -\left[ \mathbf{R}^T[\boldsymbol{\omega}_1 \times]\mathbf{q} \quad \mathbf{R}^T[\boldsymbol{\omega}_2 \times]\mathbf{q} \quad \mathbf{R}^T[\boldsymbol{\omega}_3 \times]\mathbf{q} \right] =$$
$$= \mathbf{R}^T \left[ [\mathbf{q}\times]\boldsymbol{\omega}_1 \quad [\mathbf{q}\times]\boldsymbol{\omega}_2 \quad [\mathbf{q}\times]\boldsymbol{\omega}_3 \right] = \mathbf{R}^T [\mathbf{q}\times] \left[ \boldsymbol{\omega}_1 \quad \boldsymbol{\omega}_2 \quad \boldsymbol{\omega}_3 \right] = \mathbf{R}^T [\mathbf{q}\times] \boldsymbol{\Omega}.$$

Thus

(A24) $$\mathbf{x}_p \equiv \frac{\partial \mathbf{x}}{\partial \mathbf{p}} = \frac{\partial [\mathbf{R}^T(\bar{\mathbf{x}} + \bar{\mathbf{d}})]}{\partial \mathbf{p}} = \left[ \frac{\partial [\mathbf{R}^T(\bar{\mathbf{x}} + \bar{\mathbf{d}})]}{\partial \boldsymbol{\theta}} \quad \frac{\partial (\mathbf{R}^T \bar{\mathbf{d}})}{\partial \bar{\mathbf{d}}} \quad \mathbf{R}^T \frac{\partial \bar{\mathbf{x}}}{\partial \boldsymbol{\alpha}} \right] =$$
$$= \left[ \mathbf{R}^T [(\bar{\mathbf{x}} + \bar{\mathbf{d}})\times]\boldsymbol{\Omega} \quad \mathbf{R}^T \quad \mathbf{R}^T \mathbf{D} \right] = \mathbf{R}^T \left[ [(\bar{\mathbf{x}} + \bar{\mathbf{d}})\times]\boldsymbol{\Omega} \quad \mathbf{I} \quad \mathbf{D} \right],$$

where

(A25) $$\mathbf{D} \equiv \frac{\partial \bar{\mathbf{x}}}{\partial \boldsymbol{\alpha}} = \left[ \frac{\partial \bar{\mathbf{x}}}{\partial \alpha_X} \quad \frac{\partial \bar{\mathbf{x}}}{\partial \alpha_Y} \quad \frac{\partial \bar{\mathbf{x}}}{\partial \alpha_Z} \right] = \begin{bmatrix} \cos u \sin v & 0 & 0 \\ 0 & \sin u \sin v & 0 \\ 0 & 0 & \cos v \end{bmatrix}.$$

For the specific values of $\boldsymbol{\Omega} = [\boldsymbol{\omega}_1\, \boldsymbol{\omega}_2\, \boldsymbol{\omega}_3]$ we find the partials of

$\mathbf{R} = \mathbf{R}_3(\theta_3)\mathbf{R}_2(\theta_2)\mathbf{R}_1(\theta_1)$ using the well-known differentiation relations $\frac{\partial}{\partial\theta_k}\mathbf{R}_k(\theta_k) = -[\mathbf{i}_k\times]\mathbf{R}_k(\theta_k) = -\mathbf{R}_k(\theta_k)[\mathbf{i}_k\times]$, $k=1,2,3$, where $\mathbf{i}_k$ are the columns of the $3\times3$ identity matrix $\mathbf{I}_3 = [\mathbf{i}_1\ \mathbf{i}_2\ \mathbf{i}_3]$, as well as the property $[(\mathbf{Q}\mathbf{y})\times] = \mathbf{Q}[\mathbf{y}\times]\mathbf{Q}^T$ for any orthogonal $\mathbf{Q}$. Thus

(A26) $$\frac{\partial\mathbf{R}}{\partial\theta_1} = -\mathbf{R}_3(\theta_3)\mathbf{R}_2(\theta_2)[\mathbf{i}_1\times]\mathbf{R}_1(\theta_1) = -\mathbf{R}_3(\theta_3)\mathbf{R}_2(\theta_2)[\mathbf{i}_1\times]\mathbf{R}_2(-\theta_2)\mathbf{R}_3(-\theta_3)\mathbf{R} = = -[\{\mathbf{R}_3(\theta_3)\mathbf{R}_2(\theta_2)\mathbf{i}_1\}\times]\mathbf{R},$$

(A27) $$\frac{\partial\mathbf{R}}{\partial\theta_2} = -\mathbf{R}_3(\theta_3)[\mathbf{i}_2\times]\mathbf{R}_2(\theta_2)\mathbf{R}_1(\theta_1) = = -\mathbf{R}_3(\theta_3)[\mathbf{i}_2\times]\mathbf{R}_3(-\theta_3)\mathbf{R}_3(\theta_3)\mathbf{R}_2(\theta_2)\mathbf{R}_1(\theta_1) = -[\{\mathbf{R}_3(\theta_3)\mathbf{i}_2\}\times]\mathbf{R}_3(-\theta_3)\mathbf{R},$$

(A28) $$\frac{\partial\mathbf{R}}{\partial\theta_2} = -[\mathbf{i}_3\times]\mathbf{R}_3(\theta_3)\mathbf{R}_2(\theta_2)\mathbf{R}_1(\theta_1) = -[\mathbf{i}_3\times]\mathbf{R},$$

while from $[\boldsymbol{\omega}_k\times] = \frac{\partial\mathbf{R}}{\partial\theta_k}\mathbf{R}^T$ it follows that

(A29) $$\boldsymbol{\omega}_1 = -\mathbf{R}_3(\theta_3)\mathbf{R}_2(\theta_2)\mathbf{i}_1,\ \boldsymbol{\omega}_2 = -\mathbf{R}_3(\theta_3)\mathbf{i}_2,\ \boldsymbol{\omega}_3 = -\mathbf{i}_3,$$

(A30) $$\boldsymbol{\Omega}(\boldsymbol{\theta}) = \begin{bmatrix} -\cos\theta_3\cos\theta_2 & -\sin\theta_3 & 0 \\ -\sin\theta_3\cos\theta_2 & -\cos\theta_3 & 0 \\ -\sin\theta_2 & 0 & -1 \end{bmatrix}.$$

<u>Orthogonal projection of a point on the surface of the ellipsoid.</u>

In order to project a given point on the surface of an ellipsoid with known parameters, we can always convert the point coordinates to the ellipsoid aligned reference system, where it satisfies $\mathbf{x}^T\boldsymbol{\Lambda}\mathbf{x} = 1$ ($\boldsymbol{\Lambda}$ diagonal with $\Lambda_{11} = 1/\alpha_X^2$, $\Lambda_{22} = 1/\alpha_Y^2$, $\Lambda_{33} = 1/\alpha_Z^2$)). If $\mathbf{x}'$ are the converted given point coordinates in the same reference system we seek a point $\mathbf{x}$ satisfying $f(\mathbf{x}) = \mathbf{x}^T\boldsymbol{\Lambda}\mathbf{x} - 1 = 0$, such that $\mathbf{x} - \mathbf{x}' = \rho\mathbf{g}(\mathbf{x})$, where $\mathbf{g} = \mathit{grad}f = 2\boldsymbol{\Lambda}\mathbf{x}$. Therefore $\mathbf{x} - \mathbf{x}' = \rho\mathbf{g}(\mathbf{x}) = 2\rho\boldsymbol{\Lambda}\mathbf{x}$, which yields $\mathbf{x} = (\mathbf{I} - 2\rho\boldsymbol{\Lambda})^{-1}\mathbf{x}'$. Replacing this in $f(\mathbf{x})$ we obtain the following nonlinear equation in $\rho$

(A31) $$\mathbf{x}'^T(\mathbf{I} - 2\rho\boldsymbol{\Lambda})^{-1}\boldsymbol{\Lambda}(\mathbf{I} - 2\rho\boldsymbol{\Lambda})^{-1}\mathbf{x}' - 1 = 0.$$

Since $\mathbf{I} - 2\rho\boldsymbol{\Lambda}$ is diagonal with elements $(\mathbf{I} - 2\rho\boldsymbol{\Lambda})_{ii} = 1 - 2\rho\Lambda_{ii}$, the inverse will have diagonal elements $1/(1 - 2\rho\Lambda_{ii})$ and $[(\mathbf{I} - 2\rho\boldsymbol{\Lambda})^{-1}\boldsymbol{\Lambda}(\mathbf{I} - 2\rho\boldsymbol{\Lambda})^{-1}]_{ii} = = \Lambda_{ii}/(1 - 2\rho\Lambda_{ii})^2$. Thus the explicit form of the above equation becomes

$$\sum_{i=1}^{3} x_i'^2 \frac{\Lambda_{ii}}{(1-2\rho\Lambda_{ii})^2} - 1 = 0 \text{ or with } x_i' = [X_i' \; Y_i' \; Z_i']^T$$

(A32)
$$\left(\frac{X'\alpha_X}{\alpha_X^2 - 2\rho}\right)^2 + \left(\frac{Y'\alpha_Y}{\alpha_Y^2 - 2\rho}\right)^2 + \left(\frac{Z'\alpha_Z}{\alpha_Z^2 - 2\rho}\right)^2 - 1 = 0$$

This is a nonlinear equation (equivalent to a 6th order polynomial in $\rho$) that can be solved by any of the relevant standard methods of numerical analysis. Once $\rho$ is determined the desired projection is computed from $\mathbf{x} = (\mathbf{I} - 2\rho\mathbf{\Lambda})^{-1}\mathbf{x}'$, explicitly

(A33)
$$\mathbf{x} = \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} = \begin{bmatrix} \dfrac{\alpha_X^2}{\alpha_X^2 - 2\rho} X' \\ \dfrac{\alpha_Y^2}{\alpha_Y^2 - 2\rho} Y' \\ \dfrac{\alpha_Z^2}{\alpha_Z^2 - 2\rho} Z' \end{bmatrix}.$$

Finally the distance $r = \| \mathbf{x}' - \mathbf{x} \|$ can be computed by combining $\mathbf{x} - \mathbf{x}' = 2\rho\mathbf{\Lambda}\mathbf{x}$ with $\mathbf{x} = (\mathbf{I} - 2\rho\mathbf{\Lambda})^{-1}\mathbf{x}'$ to get $\mathbf{x} - \mathbf{x}' = 2\rho\mathbf{\Lambda}(\mathbf{I} - 2\rho\mathbf{\Lambda})^{-1}\mathbf{x}'$, so that $r^2 = (\mathbf{x} - \mathbf{x}')^T(\mathbf{x} - \mathbf{x}') = 4\rho^2\mathbf{x}'(\mathbf{I} - 2\rho\mathbf{\Lambda})^{-1}\mathbf{\Lambda}^2(\mathbf{I} - 2\rho\mathbf{\Lambda})^{-1}\mathbf{x}'$, or explicitly

(A34)
$$r = 2\rho\sqrt{\left(\frac{X'}{\alpha_X^2 - 2\rho}\right)^2 + \left(\frac{Y'}{\alpha_Y^2 - 2\rho}\right)^2 + \left(\frac{Z'}{\alpha_Z^2 - 2\rho}\right)^2}.$$

The above algorithm is adapted from Spain et al. (1960), Ch. V-40, p. 43 and was reproduced by Hart (2006) and Eberly (2013). More complicated approaches have been proposed by Bektas (2014a, 2014b). For an iterative approach see Hu & Wallner (2005).

## Appendix B: Adjustment of observation equations with constraints containing additional parameters

Consider the linear model $\mathbf{b} = \mathbf{A}\mathbf{x} + \mathbf{e}$ with constraints $\mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{y} + \mathbf{d} = \mathbf{0}$, which contain additional parameters $\mathbf{y}$. To find the least squares solution, $\mathbf{e}^T\mathbf{P}\mathbf{e} = (\mathbf{b} - \mathbf{A}\mathbf{x})^T\mathbf{P}(\mathbf{b} - \mathbf{A}\mathbf{x}) = \min$, under these constraints we form the Lagrangean

(B1)
$$\Phi = (\mathbf{b} - \mathbf{A}\mathbf{x})^T\mathbf{P}(\mathbf{b} - \mathbf{A}\mathbf{x}) + 2\mathbf{k}^T(\mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{y} + \mathbf{d}),$$

and we set its derivatives with respect to the unknowns and the Lagrange multipliers $\mathbf{k}$ equal to zero

(B2) $$\frac{\partial \Phi}{\partial \mathbf{x}} = -2(\mathbf{b} - \mathbf{A}\hat{\mathbf{x}})^T \mathbf{P}\mathbf{A} + 2\mathbf{k}^T \mathbf{C} = \mathbf{0},$$

(B3) $$\frac{\partial \Phi}{\partial \mathbf{y}} = 2\mathbf{k}^T \mathbf{D} = \mathbf{0},$$

(B4) $$\frac{\partial \Phi}{\partial \mathbf{k}} = 2(\mathbf{C}\hat{\mathbf{x}} + \mathbf{D}\hat{\mathbf{y}} + \mathbf{d})^T = \mathbf{0}.$$

The solution is provided by the linear system

(B5) $$\mathbf{A}^T \mathbf{P}\mathbf{A}\hat{\mathbf{x}} - \mathbf{C}^T \mathbf{k} = \mathbf{A}^T \mathbf{P}\mathbf{b},$$

(B6) $$\mathbf{D}^T \mathbf{k} = \mathbf{0},$$

(B7) $$\mathbf{C}\hat{\mathbf{x}} + \mathbf{D}\hat{\mathbf{y}} + \mathbf{d} = \mathbf{0}$$

Setting $\mathbf{N} = \mathbf{A}^T \mathbf{P}\mathbf{A}$ and $\mathbf{u} = \mathbf{A}^T \mathbf{P}\mathbf{b}$ we may solve (B5) for $\hat{\mathbf{x}} = \mathbf{N}^{-1}\mathbf{u} + \mathbf{N}^{-1}\mathbf{C}^T \mathbf{k}$, replace this in (B7) and solve for

(B8) $$\mathbf{k} = -(\mathbf{C}\mathbf{N}^{-1}\mathbf{C}^T)^{-1}(\mathbf{D}\hat{\mathbf{y}} + \mathbf{d}) - (\mathbf{C}\mathbf{N}^{-1}\mathbf{C}^T)^{-1}\mathbf{C}\mathbf{N}^{-1}\mathbf{u},$$

which replaced in (B6) gives

(B9) $$\mathbf{D}^T(\mathbf{C}\mathbf{N}^{-1}\mathbf{C}^T)^{-1}(\mathbf{D}\hat{\mathbf{y}} + \mathbf{d}) - \mathbf{D}^T(\mathbf{C}\mathbf{N}^{-1}\mathbf{C}^T)^{-1}\mathbf{C}\mathbf{N}^{-1}\mathbf{u} = \mathbf{0}.$$

This can be solved for

(B10) $$\hat{\mathbf{y}} = -\left[\mathbf{D}^T(\mathbf{C}\mathbf{N}^{-1}\mathbf{C}^T)^{-1}\mathbf{D}\right]^{-1}\mathbf{D}^T(\mathbf{C}\mathbf{N}^{-1}\mathbf{C}^T)^{-1}(\mathbf{C}\mathbf{N}^{-1}\mathbf{u} + \mathbf{d}).$$

Replacing from (B8) into $\hat{\mathbf{x}} = \mathbf{N}^{-1}\mathbf{u} + \mathbf{N}^{-1}\mathbf{C}^T \mathbf{k}$ gives

(B11) $$\hat{\mathbf{x}} = \mathbf{N}^{-1}\mathbf{u} - \mathbf{N}^{-1}\mathbf{C}^T(\mathbf{C}\mathbf{N}^{-1}\mathbf{C}^T)^{-1}(\mathbf{C}\mathbf{N}^{-1}\mathbf{u} + \mathbf{d}) - \mathbf{N}^{-1}\mathbf{C}^T(\mathbf{C}\mathbf{N}^{-1}\mathbf{C}^T)^{-1}\mathbf{D}\hat{\mathbf{y}},$$

or utilizing the value of $\hat{\mathbf{y}}$ from (B10)

(B12) $$\hat{\mathbf{x}} = \mathbf{N}^{-1}\mathbf{u} - \mathbf{N}^{-1}\mathbf{C}^T(\mathbf{C}\mathbf{N}^{-1}\mathbf{C}^T)^{-1}(\mathbf{C}\mathbf{N}^{-1}\mathbf{u} + \mathbf{d}) +$$
$$+\mathbf{N}^{-1}\mathbf{C}^T(\mathbf{C}\mathbf{N}^{-1}\mathbf{C}^T)^{-1}\mathbf{D}\left[\mathbf{D}^T(\mathbf{C}\mathbf{N}^{-1}\mathbf{C}^T)^{-1}\mathbf{D}\right]^{-1}\mathbf{D}^T(\mathbf{C}\mathbf{N}^{-1}\mathbf{C}^T)^{-1}(\mathbf{C}\mathbf{N}^{-1}\mathbf{u} + \mathbf{d}).$$

We need only (B10) and (B11) for a sequential solution to the least squares problem.

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