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Determination of fabric and strain ellipsoids from measured sectional ellipses — theory

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Abstract

Calculating a 'fabric ellipsoid' from sectional fabric ellipses is a common requirement in studies of rock fabrics. There may be any number, $N \geq 3$ of sections, with arbitrary orientations, and absolute or relative sizes of the sectional ellipses are often not known. In the method presented here, the solution is shown to be that of a system of linear equations, and that solution can always be found. An 'incompatibility index' permits an assessment of how well sectional data fit with each other, and allowance can also be made for different levels of confidence for the different sectional ellipses.

Keywords: Fabric ellipsoid; Incompatibility index; Sectional ellipses

1. Introduction

When collecting fabric data from the rocks they study, geologists generally seek three-dimensional information. However, many fabric data can only be conveniently collected on planar section, and combining fabric data from several planar sections into three-dimensional fabric information is required. The present contribution is only concerned with orthorhombic fabric information — such as grain, aggregate or pebble shape fabrics, or strain fabrics — that can be described, at least in part by ellipsoids. The task of the geologist is then to infer an ellipsoid from sectional ellipses that are measured on planar sections. While a large fraction of the literature on this topic has been focused on paleostrain analysis, the problem and its solution are applicable to many other fabrics that may be related to the primary formation of a rock rather than its strain.

Ramsay (1967) was the first to discuss the calculation of three-dimensional strain from sections that are not parallel to the principal planes of strain. The present review is restricted to those methods, sometimes described as 'matrix methods', or 'eigenvector methods', which determine algebraic parameters for the ellipsoid. Shimamoto and Ikeda (1976, pp. 330–333) proposed an approximate solution to that problem for the special case when strain measurements are available on three orthogonal sections. Oertel (1978), also concerned with three orthogonal sections, introduced the notion of 'observational error' assigned to the parameters describing individual elliptical markers measured in each face, and noted that the parameters of the 'best-fitting' average ellipsoid had to minimise the total error. Miller and Oertel (1979), with significant corrections to Oertel's (1978) original theory, presented an implementation of it; the method involved the calculation of two successive sets of 'residuals' for each of the three faces. Although still restricted to three faces, Milton (1980) proposed a method that could be used when these faces are not perpendicular to each other. That author introduced the concept of 'adjustment strain ellipse', and used a Mohr circle representation to justify the choice of one among an infinite family of possible such ellipses. Gendzwill and Stauffer (1981) and Shao and Wang (1984) proposed a method similar to that of Shimamoto and Ikeda but allowed for non-perpendicular faces. Shao and Wang (1984) also proposed a least-square solution for data from more than three sections. All the above authors dealt with the problem of size of the sectional ellipse, described below, by scaling these sizes separately from finding the best ellipsoid. Owens (1984) was the first author to propose a method of ellipsoid determination from ellipses measured on any number of faces that tackled sectional ellipse sizes and ellipsoid determination together. However, Owens' matrix equation did not separate the parameters sought from the data, and an iterative procedure, starting from a trial solution, was thus still necessary to find a 'best-fit' solution. None of the algorithms proposed so far are completely robust.

The present contribution demonstrates a direct, non-

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iterative method for calculating an ellipsoid from the knowledge of sectional ellipses measured on any sufficient (i.e. ≥3) number of faces having any arbitrary orientations. Minimising the sum of *norms* of 'error matrices' defined for each measured face does lead to a set of linear equations for the six independent parameters of the ellipsoid sought. One only needs to enter measured data to calculate the coefficients of a system of linear equations, which is then readily solved. The method involves no iteration, and works every time. When the solution corresponds to a hyperboloid rather than an ellipsoid, it is because the data themselves are poor or insufficient and best fit a hyperboloid. Compatibility of the data is readily assessed, and account can be taken of varying reliabilities of measurements from different faces. The method has been fully tested with ELLIPSOID, a Visual Basic program, and examples of results are presented by Launeau and Robin (in preparation).

Physical properties that are described by second-rank tensor properties (e.g. thermal expansion, thermal and electrical conductivity, magnetic susceptibility) are commonly determined from measurements of these properties along a sufficient number of line directions. The calculation of the full tensor amounts to finding the coefficients of the three-dimensional tensor that best fit these one-dimensional measurements. The six independent tensor components sought are solutions to a system of six linear equations, the coefficients of these equations being functions of the measurement data. Because the solution is normally found numerically by inversion of the matrix of coefficients of this system of equations (e.g. Nye, 1957, Chap. 9), such methods are described as 'matrix inversion methods'. This paper presents a similar matrix inversion method for the case when sectional measurements yield sectional ellipses, as opposed to the scalar data obtained from measurements along line directions.

However, determinations of second-rank tensor physical properties rely on the fact that absolute measurements of these properties can be made along a sufficient number of specific directions. In contrast, when determining fabric ellipsoids from sectional ellipses, one cannot always measure absolute sizes of these ellipses. Two cases must therefore be distinguished. In *Case 1*, the sectional ellipses do have measured sizes, which differ from section to section. Launeau and Robin (in preparation) provide examples in which areas of sectional fabric ellipses are sometimes accessible. By ignoring this latter case, geologists may fail to take advantage of the full information available. In the more common *Case 2*, measurements only yield directions and axial ratios of sectional ellipses.

2. Representation of the fabric ellipsoid by an 'inverse shape matrix'

The present method, like those of Shimamoto and Ikeda (1976) and of other authors reviewed above, is based on the description of an ellipsoid by its quadratic equation and its corresponding quadratic form matrix. The general equation of an ellipsoid, in a specified common reference coordinate system (of axes 1, 2, and 3), can indeed be expressed by a quadratic equation:

$$b_{11}x_1x_1 + b_{22}x_2x_2 + b_{33}x_3x_3 + 2b_{23}x_2x_3 + 2b_{13}x_1x_3 + 2b_{12}x_1x_2 = 1 \quad \text{(1a)}$$

where x_1, x_2, and x_3 are coordinates of a point that is on the ellipsoid if Eq. (1) is satisfied. In matrix form:

$$\mathbf{X}^{\mathrm{T}}\mathbf{B}\mathbf{X} = 1 \quad \text{(1b)}$$

where

$$\mathbf{X} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \text{ and } \mathbf{X}^{\mathrm{T}} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}$$

(a superscript T denotes a transposed matrix), and **B** is a real symmetric 3 × 3 matrix:

$$\mathbf{B} = \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{12} & b_{22} & b_{23} \\ b_{13} & b_{23} & b_{33} \end{bmatrix} \quad (2)$$

Shimamoto and Ikeda (1976) called the matrix **B** the 'shape matrix' of the ellipsoid. But because its principal values are inverse functions of the lengths of the corresponding diameters of the ellipsoid (see Eq. (3) below), Wheeler's (1986) name of 'inverse shape matrix' is used here. For a quadratic equation to represent an ellipsoid, rather than, e.g. a hyperboloid, or an elliptical cylinder, the eigenvalues of its matrix, $b_1 > b_2 > b_3$, must all be positive numbers. The directions of the major, intermediate, and minor semi-diameters of the ellipsoid are the same as those of the eigenvectors of **B**, and their dimensions, A^{d}, B^{d}, and C^{d}, are given by:

$$A^{\mathrm{d}} = \frac{1}{\sqrt{b_3}}, \qquad B^{\mathrm{d}} = \frac{1}{\sqrt{b_2}}, \qquad C^{\mathrm{d}} = \frac{1}{\sqrt{b_1}} \quad (3)$$

3. Sectional measurements

3.1. The elliptical trace of an ellipsoid on a planar section

Sectional measurements are made on several planar sections: Face 1, Face 2, Face 3, etc. Each such face, say *I*

(Fig. 1a), is characterised by its normal vector, e.g.

$$\mathbf{l}_1^I = \begin{bmatrix} l_{11}^I \\ l_{12}^I \\ l_{13}^I \end{bmatrix}$$

and by a Cartesian coordinate system within that face

$$\mathbf{l}_2^I = \begin{bmatrix} l_{21}^I \\ l_{22}^I \\ l_{23}^I \end{bmatrix}, \mathbf{l}_3^I = \begin{bmatrix} l_{31}^I \\ l_{32}^I \\ l_{33}^I \end{bmatrix}$$

where the superscript designates the section. Each section face, in effect, defines a new coordinate system described by

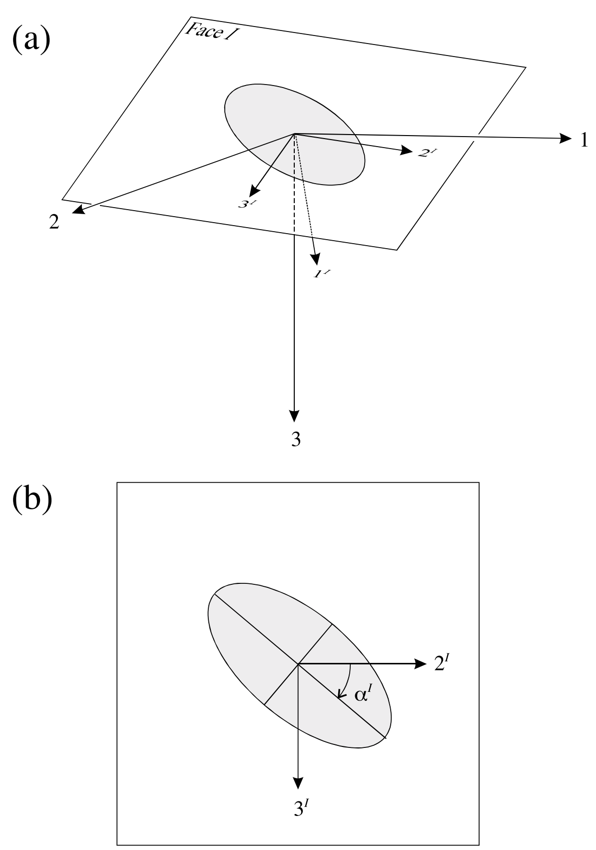

Fig. 1. (a) A fabric ellipsoid is known by its elliptical sections on three or more faces. Each face I is characterised by its own coordinate system, of axes 1^I, 2^I, and 3^I, with the 1^I-axis chosen normal to the face. The best-fit ellipsoid is the one that minimises the differences between its elliptical sections and the ellipses actually measured on all faces. (b) On each face, the ellipse is known by at least two parameters, such as the ratio R of its long to its short axis, and the angle α of its long axis with coordinate axis 2^I. In *Case 2*, these two parameters are the only information provided by the section. In *Case 1*, sections yield additional information about the relative sizes of different sections of the ellipsoid (e.g. different average areas, or different densities of markers on different sections).

the orthogonal matrix:

$$\mathbf{L}^I = \begin{bmatrix} l_{11}^I & l_{21}^I & l_{31}^I \\ l_{12}^I & l_{22}^I & l_{32}^I \\ l_{13}^I & l_{23}^I & l_{33}^I \end{bmatrix} \quad (4)$$

In this coordinate system, the inverse shape matrix of the ellipsoid is:

$$\mathbf{B}^I = \mathbf{L}^{I\mathrm{T}}\mathbf{B}\mathbf{L}^I$$

Sectional measurements for Face I only give us an ellipse (Fig. 1), specified by a 2×2 matrix that is related to $\mathbf{B}$ by:

$$\begin{bmatrix} b_{22}^I & b_{23}^I \\ b_{23}^I & b_{33}^I \end{bmatrix} = \begin{bmatrix} l_{21}^I & l_{22}^I & l_{23}^I \\ l_{31}^I & l_{32}^I & l_{33}^I \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{12} & b_{22} & b_{23} \\ b_{13} & b_{23} & b_{33} \end{bmatrix} \times \begin{bmatrix} l_{21}^I & l_{31}^I \\ l_{22}^I & l_{32}^I \\ l_{23}^I & l_{33}^I \end{bmatrix} + \begin{bmatrix} \chi_{22}^I & \chi_{23}^I \\ \chi_{23}^I & \chi_{33}^I \end{bmatrix} \quad (5)$$

The 2×2 matrix $\mathbf{X}^I$ is the error associated with our measurement on Face I. For each face, $\mathbf{X}^I$ represents, in a way, Milton's (1980) 'adjustment ellipse'. We can rewrite it:

$$\begin{bmatrix} \chi_{22}^I & \chi_{23}^I \\ \chi_{23}^I & \chi_{33}^I \end{bmatrix} = \begin{bmatrix} b_{22}^I & b_{23}^I \\ b_{23}^I & b_{33}^I \end{bmatrix} - \begin{bmatrix} l_{21}^I & l_{22}^I & l_{23}^I \\ l_{31}^I & l_{32}^I & l_{33}^I \end{bmatrix} \times \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{12} & b_{22} & b_{23} \\ b_{13} & b_{23} & b_{33} \end{bmatrix} \begin{bmatrix} l_{21}^I & l_{31}^I \\ l_{22}^I & l_{32}^I \\ l_{23}^I & l_{33}^I \end{bmatrix} \quad (6)$$

We note that $\mathbf{X}^I$, being a deviation from some expected value, can be described as the matrix equivalent of a deviation from a mean for a scalar parameter. We can anticipate that a sum of *norms* of such matrices for all faces measured will have to be minimised by the best-fit solution; the *norm* of a matrix is a scalar parameter that describes the 'magnitude' of that matrix.

But before using Eq. (6), we must discuss the amount of information that may or may not be available from sectional measurements. As already stated, there are essentially two cases, referred to as Case 1 and Case 2.

3.2. Case 1: sectional measurements yield information about the size of the sectional ellipse

At least two parameters are required from each section in order to calculate an ellipsoid. These are, typically, the axial ratio of the sectional ellipse, ρ^I, and a direction, such as the angle its long axis makes with, say, the 2-axis direction for that face, α^I (Fig. 1b). In some cases, however, sections provide one more parameter that the geologist can use, namely information on an area of that sectional ellipse, or at least relative areas among variously oriented sections.

If the ellipsoid sought is a finite strain ellipsoid, there are some measurement methods, such as methods using boudinaged markers, or buckled layers, which potentially yield absolute strains. It is admittedly hard to imagine a method that could yield absolute strains in several, variously oriented sections, but it is at least possible in principle. More commonly, however, fabric indicators, whether or not they can be reliably interpreted as strain indicators, may carry unambiguous relative size information.

For example, fabric indicators are often shapes of mineral grains or mineral aggregates that have definite sectional areas as well as axial ratios. If a sufficient number of markers has been measured for each face I such that their average sectional area, $\bar{a}^I$, can be considered representative, then the three independent parameters describing the sectional ellipse can be taken as:

$$\begin{bmatrix} b^I_{22} & b^I_{23} \\ b^I_{23} & b^I_{33} \end{bmatrix} = \frac{1}{\bar{a}^I}\begin{bmatrix} \dfrac{\cos^2\alpha^I}{\rho^I} + \rho^I\sin^2\alpha^I & \left(\dfrac{1}{\rho^I} - \rho^I\right)\cos\alpha^I\sin\alpha^I \\ \left(\dfrac{1}{\rho^I} - \rho^I\right)\cos\alpha^I\sin\alpha^I & \rho^I\cos^2\alpha^I + \dfrac{\sin^2\alpha^I}{\rho^I} \end{bmatrix} = \frac{1}{\bar{a}^I}\begin{bmatrix} \hat{b}^I_{22} & \hat{b}^I_{23} \\ \hat{b}^I_{23} & \hat{b}^I_{33} \end{bmatrix} \quad (7)$$

In other words, each section for which we can measure an average area of markers yields all three components of the inverse shape matrix describing the ellipse, not just α^I and ρ^I.

In some other situations, measurements may yield the dimension of the sectional ellipse through the actual lengths of its axes. Or, if the fabric examined is a spatial distribution of markers, their respective densities, $\bar{n}^I$, in different sections also carries information:

$$\begin{bmatrix} b^I_{22} & b^I_{23} \\ b^I_{23} & b^I_{33} \end{bmatrix} = \bar{n}^I\begin{bmatrix} \hat{b}^I_{22} & \hat{b}^I_{23} \\ \hat{b}^I_{23} & \hat{b}^I_{33} \end{bmatrix} \quad (8)$$

We note incidentally that if the markers are uniformly distributed in the rock, their expected modal proportions are the same on all faces, and therefore:

$$\bar{n}^1\bar{a}^1 = \bar{n}^2\bar{a}^2 = \bar{n}^3\bar{a}^3 = \ldots \quad (9)$$

If, in such case, both measurements of marker density and average area are available, Eq. (9) provides a test of whether the faces provide reliable estimates of both.

3.3. Case 2: sectional measurements yield no information about size of sectional ellipse

There are many fabric indicators that do not yield reliable information about relative areas. For example, the number of markers on each face is insufficient to average over the 'section effect', or insufficient to measure a reliable density. The three independent components of the inverse shape matrix representing the sectional ellipse are then related to the two measured parameters by an unknown scale factor, f^I:

$$\begin{bmatrix} b^I_{22} & b^I_{23} \\ b^I_{23} & b^I_{33} \end{bmatrix} = f^I\begin{bmatrix} \hat{b}^I_{22} & \hat{b}^I_{23} \\ \hat{b}^I_{23} & \hat{b}^I_{33} \end{bmatrix} \quad (10)$$

As will be seen next, the detail of the method used to extract an ellipsoid from the sectional information depends on whether or not section faces yield areal information.

4. Calculating the ellipsoid

4.1. The Frobenius norm of the error matrix

Although the 'deviation matrix', $\mathbf{X}^I$, is a 2×2 matrix, we can assign some scalar measure of its magnitude with its *Frobenius norm*. The Frobenius norm of a matrix $\mathbf{A}$ is one of several possible ways to describe the 'magnitude' of that matrix. It is equal to $\sqrt{\sum_{i,j}(a_{ij})^2}$, where a_{ij} are components of $\mathbf{A}$, and the summation is over all the values of the indices (e.g. Goldberg, 1991, pp. 332 and ff). Note that its expression is similar to that of the magnitude of a vector. It is of course zero if all the components are zero, and, for a real symmetric matrix, it is invariant with respect to rotations of the coordinates, and, in particular, equal to the square root of the sum of the squares of its eigenvalues (e.g. Goldberg, 1991, p. 335). In the demonstration of this paper, we shall deal only with the square of the Frobenius norm; we shall refer to it as the 'squared Frobenius norm', or the 'squared norm', and designate it by F (even when it is declared, as in Eq. (11), as a single component matrix).

We noted earlier that $\mathbf{X}^I$ was the matrix equivalent of a deviation; its squared Frobenius norm, F^I, is the equivalent of a second moment. In order to highlight the dependence of F^I on the independent components of $\mathbf{B}$, which we seek, it can be expressed in the form of the 1×1 matrix product

(Appendix A):

$$F^I = [\, b_{11} \quad b_{22} \quad b_{33} \quad b_{23} \quad b_{13} \quad b_{12} \,] \times \left\{ \mathbf{R}^I \begin{bmatrix} b_{11} \\ b_{22} \\ b_{33} \\ b_{23} \\ b_{13} \\ b_{12} \end{bmatrix} - 2\,\mathbf{S}^I \right\} + \mathbf{T}^I \tag{11}$$

where: $\mathbf{R}^I$ is a 6×6 symmetric matrix (Eq. (A5)), of rank three (Appendix A, Section A.1.1.1), which is a function only of the orientation of the normal to the section; $\mathbf{S}^I$ is 1×6 column matrix (Eq. (A6)), which is a mixed function of the orientation of the coordinate axes in the section and of the two measured parameters of the sectional ellipse; and $\mathbf{T}^I$ is a 1×1 matrix of component equal to the squared Frobenius norm of the inverse shape matrix of the measured sectional ellipse (Eq. (A7)).

4.2. Combining sectional traces to obtain the ellipsoid

When we have measurements on faces $I = 1, 2,\ldots,N$, and, assuming for now that we have equal confidence in the measurements from all sections, we can define the sum, F, of the squared Frobenius norms of the error matrices for all N faces:

$$F = \sum_{I=1}^{N} F^I = [\, b_{11} \quad b_{22} \quad b_{33} \quad b_{23} \quad b_{13} \quad b_{12} \,] \times \left\{ \mathbf{R} \begin{bmatrix} b_{11} \\ b_{22} \\ b_{33} \\ b_{23} \\ b_{13} \\ b_{12} \end{bmatrix} - 2\mathbf{S} \right\} + \mathbf{T} \tag{12}$$

where

$$\mathbf{R} = \sum_{I=1}^{N} \mathbf{R}^I \tag{13}$$

$$\mathbf{S} = \sum_{I=1}^{N} \mathbf{S}^I \tag{14}$$

and

$$\mathbf{T} = \sum_{I=1}^{N} \mathbf{T}^I \tag{15}$$

R, **S**, and **T**, like their contributing matrices, are respectively 6×6, 1×6, and 1×1 matrices, obtained by summing individual components of their contributors. But whereas each $\mathbf{R}^I$ is of rank three, their sum **R** is of rank six, provided faces have three or more different orientations.

The components of **B** that best fit the measurements are those for which F is minimum. Note that F is a parabolic function of each of the independent components of **B**. Let us examine how to calculate them for the two cases discussed earlier.

4.3. Case 1: sectional measurements yield areal information

4.3.1. General case of several non-orthogonal sections

We seek the values of the six independent components of **B** such that the partial derivatives of F with respect to each one of them are all zero. Since F is a quadratic expression of these components, its derivatives are linear in them, and they therefore must satisfy a system of six linear equations. This system can be expressed in matrix form:

$$\begin{bmatrix} \partial F/\partial b_{11} \\ \partial F/\partial b_{22} \\ \partial F/\partial b_{33} \\ \partial F/\partial b_{23} \\ \partial F/\partial b_{13} \\ \partial F/\partial b_{12} \end{bmatrix} \equiv 2\,\mathbf{R} \begin{bmatrix} b_{11} \\ b_{22} \\ b_{33} \\ b_{23} \\ b_{13} \\ b_{12} \end{bmatrix} - 2\,\mathbf{S} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{16a}$$

or

$$\mathbf{R} \begin{bmatrix} b_{11} \\ b_{22} \\ b_{33} \\ b_{23} \\ b_{13} \\ b_{12} \end{bmatrix} = \mathbf{S} \tag{16b}$$

or

$$\begin{bmatrix} b_{11} \\ b_{22} \\ b_{33} \\ b_{23} \\ b_{13} \\ b_{12} \end{bmatrix} = \mathbf{R}^{-1}\mathbf{S} \tag{17}$$

The solution is thus obtained simply by solving Eq. (16), or by inverting the 6×6 matrix **R**. Since **R** is a real symmetric matrix, and, provided faces of at least three different orientations contribute to it, is of rank six, a solution can always be found.

Having obtained the components of **B**, one can then diagonalise it to find its eigenvalues (b_1, b_2, b_3) and eigenvectors. If the ellipsoid sought is a strain ellipsoid, absolute strain measurements would permit calculation of a volume change by any of the formulae below:

$$\frac{V'}{V} = A^{\mathrm{d}}B^{\mathrm{d}}C^{\mathrm{d}} = \frac{1}{\sqrt{\det\mathbf{B}}} \tag{18}$$

with

$$\det\mathbf{B} = b_{11}b_{22}b_{33} + 2b_{23}b_{13}b_{12} - b_{11}(b_{23})^2 - b_{22}(b_{13})^2 - b_{33}(b_{12})^2 = b_1 b_2 b_3 \tag{19}$$

4.3.2. Special case of three orthogonal sections

For many good reasons, geologists try to study rock fabrics in mutually orthogonal sections. Unless one is certain to have identified the symmetry planes of the fabric ellipsoid sought, and has cut the rock along these symmetry planes, one needs a minimum of three sections to determine that ellipsoid. If one uses software that treats the general case, the special formulae developed below are not really needed. But that development is presented here nevertheless because it yields results that can be recognised as correct from elementary considerations, and it therefore justifies the method used.

Without loss of generality we can choose a Cartesian coordinate system with axes perpendicular to each of the three sections. Choosing for each face a coordinate system such as shown in Fig. 2, the orthogonal matrices describing the orientations of the three sections are, for faces perpendicular to X, Y, and Z directions, respectively:

$$\mathbf{L}^1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{20a}$$

$$\mathbf{L}^2 = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \tag{20b}$$

$$\mathbf{L}^3 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \tag{20c}$$

The expressions of F^I then simplify to

$$F^1 = (b_{22})^2 + (b_{33})^2 + 2(b_{23})^2 - 2(b^1_{22}b_{22} + b^1_{33}b_{33} + 2b^1_{23}b_{23}) + (b^1_{22})^2 + 2(b^1_{23})^2 + (b^1_{33})^2 \tag{21a}$$

$$F^2 = (b_{11})^2 + (b_{33})^2 + 2(b_{13})^2 - 2(b^2_{22}b_{33} + b^2_{33}b_{11} + 2b^2_{23}b_{13}) + (b^2_{22})^2 + 2(b^2_{23})^2 + (b^2_{33})^2 \tag{21b}$$

$$F^3 = (b_{11})^2 + (b_{22})^2 + 2(b_{12})^2 - 2(b^3_{22}b_{11} + b^3_{33}b_{22} + 2b^3_{23}b_{12}) + (b^3_{22})^2 + 2(b^3_{23})^2 + (b^3_{33})^2 \tag{21c}$$

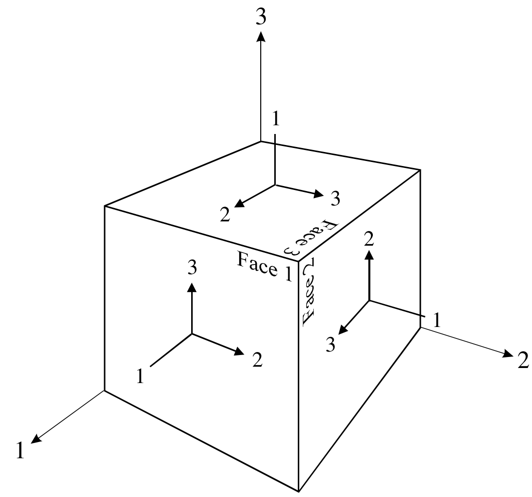

Fig. 2. Orientations of axes on three orthogonal faces used in Eqs. (20) and (21) and Table 1. These orientations have been chosen to bring out the symmetry in the results. In order to calculate ellipsoid parameters with formulae in Table 1, sectional data must be converted to correspond to these orientations.

Assuming that we have equal confidence in data from all three faces, the solution that minimizes the 'squared Frobenius sum' can be obtained by equating the derivatives of the sum of all three quantities with respect to each component of **B**. The solution to the resulting system of six linear equations in six unknowns is shown in Table 1, together with an 'incompatibility index', $\tilde{F}$, discussed in a later section.

As in the general case, the symmetry axes and dimensions of the ellipsoid can then be obtained by diagonalisation of **B**.

Table 1
Ellipsoid parameters from sectional measurements for three orthogonal faces, Case 1

$b_{11} = (b^2_{33} + b^3_{22})/2$	$b_{22} = (b^1_{22} + b^3_{33})/2$	$b_{33} = (b^1_{33} + b^2_{22})/2$
$b_{23} = b^1_{23}$	$b_{13} = b^2_{23}$	$b_{12} = b^3_{23}$
$\tilde{F} = \frac{1}{6}\frac{(b^2_{33} - b^3_{22})^2 + (b^1_{22} - b^3_{33})^2 + (b^1_{33} - b^2_{22})^2}{(b_1)^2 + (b_2)^2 + (b_3)^2}$		

4.4. Case 2: when sectional measurements do not yield area information

The error tensor for face I can be rewritten as:

$$\begin{bmatrix} \chi^I_{22} & \chi^I_{23} \\ \chi^I_{23} & \chi^I_{33} \end{bmatrix} = f^I \begin{bmatrix} \hat{b}^I_{22} & \hat{b}^I_{23} \\ \hat{b}^I_{23} & \hat{b}^I_{33} \end{bmatrix} - \begin{bmatrix} l^I_{21} & l^I_{22} & l^I_{23} \\ l^I_{31} & l^I_{32} & l^I_{33} \end{bmatrix} \times \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{12} & b_{22} & b_{23} \\ b_{13} & b_{23} & b_{33} \end{bmatrix} \begin{bmatrix} l^I_{21} & l^I_{31} \\ l^I_{22} & l^I_{32} \\ l^I_{23} & l^I_{33} \end{bmatrix} \tag{22}$$

Its squared Frobenius norm can be rewritten as Eq. (B4) (Appendix B).

Assuming again equal confidence in measurements from all faces, the 'squared Frobenius sum' for all faces can be written as the quadratic form (Appendix B):

$$F = \begin{bmatrix} b_{11} & b_{22} & b_{33} & b_{23} & b_{13} & b_{12} & f^1 & f^2 & f^3 & \cdots & f^N \end{bmatrix}$$

$$\times \left[\begin{array}{cccccc|ccccc} R_{11} & R_{12} & R_{13} & R_{14} & R_{15} & R_{16} & -\hat{S}_1^1 & -\hat{S}_1^2 & -\hat{S}_1^3 & \cdots & -\hat{S}_1^N \\ R_{12} & R_{22} & R_{23} & R_{24} & R_{25} & R_{26} & -\hat{S}_2^1 & -\hat{S}_2^2 & -\hat{S}_2^3 & \cdots & -\hat{S}_2^N \\ R_{13} & R_{23} & R_{33} & R_{34} & R_{35} & R_{36} & -\hat{S}_3^1 & -\hat{S}_3^2 & -\hat{S}_3^3 & \cdots & -\hat{S}_3^N \\ R_{14} & R_{24} & R_{34} & R_{44} & R_{45} & R_{46} & -\hat{S}_4^1 & -\hat{S}_4^2 & -\hat{S}_4^3 & \cdots & -\hat{S}_4^N \\ R_{15} & R_{25} & R_{35} & R_{45} & R_{55} & R_{56} & -\hat{S}_5^1 & -\hat{S}_5^2 & -\hat{S}_5^3 & \cdots & -\hat{S}_5^N \\ R_{16} & R_{26} & R_{36} & R_{46} & R_{56} & R_{66} & -\hat{S}_6^1 & -\hat{S}_6^2 & -\hat{S}_6^3 & \cdots & -\hat{S}_6^N \\ \hline -\hat{S}_1^1 & -\hat{S}_2^1 & -\hat{S}_3^1 & -\hat{S}_4^1 & -\hat{S}_5^1 & -\hat{S}_6^1 & \hat{T}^1 & 0 & 0 & \cdots & 0 \\ -\hat{S}_1^2 & -\hat{S}_2^2 & -\hat{S}_3^2 & -\hat{S}_4^2 & -\hat{S}_5^2 & -\hat{S}_6^2 & 0 & \hat{T}^2 & 0 & \cdots & 0 \\ -\hat{S}_1^3 & -\hat{S}_2^3 & -\hat{S}_3^3 & -\hat{S}_4^3 & -\hat{S}_5^3 & -\hat{S}_6^3 & 0 & 0 & \hat{T}^3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\hat{S}_1^N & -\hat{S}_2^N & -\hat{S}_3^N & -\hat{S}_4^N & -\hat{S}_5^N & -\hat{S}_6^N & 0 & 0 & 0 & 0 & \hat{T}^N \end{array}\right] \begin{bmatrix} b_{11} \\ b_{22} \\ b_{33} \\ b_{23} \\ b_{13} \\ b_{12} \\ f^1 \\ f^2 \\ f^3 \\ \vdots \\ f^N \end{bmatrix} \quad (23)$$

The value of F is thus given by a homogeneous quadratic function of all the unknown parameters sought. Stated another way, the dependence of F on all the unknowns can be represented as a 'paraboloid' in a space of $(N+7)$ dimensions. Generally (except for a 'perfect fit', see end of Appendix B), the minimum of F is at the origin in that space, i.e. for $b_{11} = b_{22} = \ldots = b_{12} = f^1 = f^2 = \ldots = f^N = 0$.

This is of course not the solution we seek. We need to constrain the minimum by the requirement that at least one of the parameters sought differs from zero. As such a constraint, we may, for example, impose that the scale parameter for the first face, f^1, be equal to one. Or we may choose instead $f^2 = 1$. These two different constraints correspond in effect to two different sections through our paraboloid, and will accordingly lead to somewhat different values for the other parameters that minimize F along the two 'parabolic' sections. In other words, the best-fit solution found depends to some extent on how that solution is constrained, unless the fit is ideally perfect (see discussion at the end of Appendix B). Experimenting with actual data shows that the difference can be significant. Similarly, constraining the solution with $b_{11} = 1$, or $b_{22} = 1$, etc., yield, at least in principle, different solutions that depend in addition on the coordinate system chosen. Rather than arbitrarily selecting one face or another, or one particular axis of one arbitrary coordinate system, the 'symmetric' constraint chosen here is to impose that the trace of the inverse shape matrix — which trace is invariant in a change of coordinates, and is thus also the sum of its eigenvalues — be equal to three:

$$b_{11} + b_{22} + b_{33} = 3 \quad (24)$$

Finding the constrained minimum can be done with the method of Lagrange multipliers. The equivalent algorithm presented in Appendix C consists instead of using the constraint, Eq. (24), to eliminate one unknown, b_{11}. In either case, the solution is still obtained by solving a system of linear equations (Eq. (C2)).

Diagonalization of **B** gives again the dimensions and directions of the symmetry axes of the fabric ellipsoid. Whether or not that ellipsoid is a strain ellipsoid, it is common to normalise its components so that:

$$A^{\mathrm{d}} B^{\mathrm{d}} C^{\mathrm{d}} = 1 \quad (25a)$$

or

$$\det \mathbf{B} = 1. \quad (25b)$$

5. Compatibility of sectional measurements

The statistical arguments and demonstrations presented in this and the two following sections are probably not as rigorous as they should be. They are presented nevertheless because they appear reasonable, have proven to be practically useful, and may provide a start for a future, more exact analysis.

5.1. Calculation of squared Frobenius norms for individual faces and for the sample

Once a solution for **B** is found, the squared Frobenius norm for the error matrix associated with each Face I can be calculated. To that effect, we can use Eq. (11) (Case 1) or Eq. (B4) (Case 2), thus taking advantage of calculations that have already been done. With the resulting table, one can inspect which face (or faces) may fit the solution poorly and, eventually, re-examine or discard data that are deemed suspect. By normalizing to the squared Frobenius norm of **B**:

$$F^B = (b_1)^2 + (b_2)^2 + (b_3)^2 \quad (26)$$

one can compare such values among different samples.

Summing these 'normalized squared Frobenius norms' for all faces yields the 'normalized minimum squared Frobenius sum'. In order to compare it among different samples, one must further normalize it for the number of redundancies in the data, as discussed below.

5.2. Number of redundancies

In *Case 1*, we seek to determine the six independent components of the shape matrix B. Measurements on each face provide three parameters, and N faces therefore provide $3N$ parameters. Calling r the number of redundancies:

$$r = 3N - 6 \quad (27)$$

In *Case 2*, each face only provides two parameters, but the number of independent components of B that can be determined is only five, since their size is arbitrary and they are, in fact, subsequently normalized. Therefore:

$$r = 2N - 5 \quad (28)$$

Thus, for $N = 3$ faces, $r = 3$ in Case 1 and $r = 1$ in Case 2.

5.3. Incompatibility index

A good index of incompatibility of the measurements is therefore:

$$\tilde{F} = \frac{F^{\min}}{r\,F^B} = \frac{1}{r\,F^B}\sum_{I=1}^{N} F^I_{\min} \quad (29)$$

The lower the value of $\tilde{F}$, the more compatible are the data; the higher it is, the more incompatible the data. For Case 1 and three orthogonal faces, the algebraic expression for $\tilde{F}$ is given in Table 1.

$\tilde{F}$ is a ratio of squared values of the coefficients sought. It is advantageous to use an index with the dimension of a simple ratio of these coefficients, specifically $\sqrt{\tilde{F}}$. The latter quantity is then equivalent to a normalized standard deviation about a mean.

6. Allowing for different confidences in sectional data

6.1. Reliability and 'weights'

In preceding sections, all additions of the squared Frobenius norms for individual faces to calculate a 'squared Frobenius sum' assumed that information from all faces was equally reliable. If the incompatibility index, $\tilde{F}$ or $\sqrt{\tilde{F}}$, is low, this should be generally sufficient. But if that index is high, one may want to optimise the final determination of the ellipsoid by recognising that measurements on some faces are more reliable than on others. This is easily achieved by summing weighted Frobenius norms instead of unweighted ones, i.e.:

$$F = \sum_{I=1}^{N} w^I F^I \quad (30)$$

where w^I are the weights one wants to assign to each face I.

In the general case of multiple sections, this is simply done by calculating

$$\mathbf{R} = \sum_{I=1}^{N} w^I\,\mathbf{R}^I \quad (31)$$

$$\mathbf{S} = \sum_{I=1}^{N} w^I\,\mathbf{S}^I \quad (32)$$

$$\mathbf{T} = \sum_{I=1}^{N} w^I\,\mathbf{T}^I \quad (33)$$

Solving for the unknowns is then done in the same way as in the un-weighted case. As incompatibility index, one may then take, for Case 1 and Case 2, respectively:

$$\tilde{F} = \frac{N}{\sum_{I=1}^{N} w^I}\,\frac{1}{(3N-6)F^B}\sum_{I=1}^{N}\left(w^I F^I_{\min}\right) \quad (34)$$

and

$$\tilde{F} = \frac{N}{\sum_{I=1}^{N} w^I}\,\frac{1}{(2N-5)F^B}\sum_{I=1}^{N}\left(w^I F^I_{\min}\right) \quad (35)$$

6.2. About assigning weights

There are many reasons why the geologist may have more confidence in measurements from some faces than from others, and these reasons are often not easily quantifiable. For example, outline of markers may not be equally easy to trace on all faces. The very variations in the areas of markers from face to face, discussed in the presentation of Case 1, may make the shape of the smaller markers of some faces harder to assess and measure. Or the geologist may detect some heterogeneity in the marker population on some faces, making measurements on these faces accordingly less reliable. There are instances, however, when confidence in the data can be quantified. These are when the markers are drawn from a homogeneous population and the confidence interval for the parameters measured on each face is thus related to the number of markers measured on that face. A complete statistical analysis of confidence in the results is beyond the scope of this paper, but the following section is a tentative discussion of the effect of sample[1] size on weights assigned to faces. See Oertel (1978) and Robin and Torrance (1987) for discussions of statistical concepts as applied to fabric analysis.

6.3. Confidence related to sample size

Generally, as suggested by Oertel (1978, Eq. 4) and applied by Robin and Torrance (1987, Eqs. 2 and 3) for the 'diameter ratio' method (Robin, 1977), the variance, $\sigma_{\bar{b}}^2$, of the estimate of the mean, $\bar{b}$, of a measured scalar fabric parameter, b, is given, as a function of sample size, n, by:

$$\sigma_{\bar{b}}^2 = \frac{\sigma^2}{n} \tag{36}$$

in which σ is the standard deviation of the measured parameter for the population.

Let us consider the case in which each marker in a face is itself an ellipse, or at least does contribute parameters of a sectional ellipse; the sectional ellipse for the face is therefore some mean of the individual marker ellipses. Each marker, M, can then be assigned its own error matrix, $\mathbf{X}^M$, which is, as noted above, a deviation. The Frobenius norm of that matrix is a second moment. The average value of that norm is equivalent to a variance for the population of markers in that face. It is proposed here that the 'Central limit theorem' (see e.g. Robin and Torrance, 1987) applies to the mean sectional ellipse parameters calculated from the n markers: their deviation from the true mean varies normally about the true mean, with the variance of that normal distribution given by Eq. (36). When combining several faces, the best-fit solution minimises the total variance for all faces. If σ has the same value for all faces, this is achieved by assigning to each face I a weight proportional to its number n^I, of markers, i.e.:

$$w^I \propto n^I \tag{37}$$

An alternate way to look at this result is to regard each marker of a face as an individual sectional measurement within its own separate face. Thus, measuring Face 1 with n^1 markers, Face 2 with n^2 markers, etc., is equivalent to measuring n^1 faces that happen to have the same orientation as that of Face 1, n^2 faces that happen to have the orientation of Face 2, etc.

Even if individual fabric markers cannot be represented by ellipses, one might still want to take the number measured on each face as a first approximation of the weight to assign to that face.

[1] 'Sample', following Robin and Torrance (1987), is used here in its statistical sense: it means the set of markers that are measured on a given face. Elsewhere in the paper, 'sample' meant a rock providing three or more measurable faces from which one can determine an ellipsoid.

6.4. No objective estimate of variance?

When combining results that have a high incompatibility index, even if there is no objective way to assign variances for data from various faces, the geologist may have more to gain than to lose with an argument such as expressed by the following sentence. "I really believe that measurements on Faces 1, 2 and 4 are twice as 'good' as those for Faces 3 and 5, and therefore I give them double the weight".

7. Distribution of face orientations and constraints on the results

As pointed out earlier, the squared Frobenius sum is a parabolic function of each of the independent parameters of $\mathbf{B}$. More generally, if we call δb_{ij} the variations of these parameters about the solution found:

$$F - F^{\min} = \begin{bmatrix} \delta b_{11} & \delta b_{22} & \ldots & \delta b_{12} \end{bmatrix} \mathbf{R} \begin{bmatrix} \delta b_{11} \\ \delta b_{22} \\ \vdots \\ \delta b_{12} \end{bmatrix} \tag{38}$$

This is the equation of a 'paraboloid' in the 7-dimensional space defined by F vs. $b_{11}, b_{22}, \ldots, b_{12}$. The six principal curvatures of this paraboloid are the eigenvalues of $\mathbf{R}$. As pointed out in Appendix A, Section A.1.1.1), if there is only one face contributing to $\mathbf{R}$, or if all the faces have the same orientation, three of the six eigenvalues are equal to zero; similarly, if only two face orientations contribute to $\mathbf{R}$, one eigenvalue is zero. In either case, $\mathbf{R}$ cannot be inverted and the solution is therefore indeterminate. However, if there are several faces having different orientations, but these orientations are grouped into only one narrow cluster, three of the eigenvalues will be small. Corresponding principal curvatures will therefore also be small, and the corresponding linear combinations of the sought coefficients will be poorly constrained. Similarly, if faces measured fall into only two narrow orientation clusters, one eigenvalue will be low, and one linear combination of coefficients will be poorly constrained. It is therefore good to make sure that contributing faces have a good spread of orientations, so that the eigenvalues of $\mathbf{R}$, and thus the principal curvatures of the 'paraboloid', will be evenly large.

The above discussion implies that there should be a relationship between the eigenvalues of $\mathbf{R}$ and the confidence we have in the values of individual ellipsoid parameters found. Such a relationship is not explored here.

8. Discussion and conclusion

The problem of determination of a fabric ellipsoid from sectional ellipses measured on a sufficient number of faces is common in geology. The sectional fabric ellipse measured on any given face I differs, by some 'error', from sections of the ellipsoid sought. That error can be represented by an error matrix $\mathbf{X}^I$ (Eq. (5)) and by a squared norm for that error matrix, F^I (Eqs. (A3) and (11)). The best-fitting values for the parameters of the ellipsoid are therefore those that minimise F, the sum of squared norms of the error matrices for all N faces measured.

Two cases must be distinguished, depending on whether or not sectional measurements yield information on the areas of the sectional ellipses. In Case 1, sectional measurements do give information on areas, and the parameters describing the ellipsoid are the solution of a system of six linear equations (Eqs. (16) and (17)). In Case 2, in which measurements only provide an axial ratio and an angle for the sectional ellipses, ellipsoid parameters and the unknown scale factors are solutions of a system of $N+5$ linear equations (Appendix C, Eq. (C1)).

Provided that data exist for at least three different face orientations, the 'squared Frobenius sum', F, minimised by the solution only has one minimum. The method is therefore completely robust, in the sense that a best solution is always found. This is true even if the data are very incompatible. It is therefore important to quantify the incompatibility of the data: the value of F corresponding to the solution, properly normalized (Eq. (29)), readily provides such an incompatibility index. That definition can be modified to take into account the variable confidences that one might have in the sectional data (Eqs. (34) and (35)).

Implementing the method presented here is laborious (e.g. see the expressions given in the appendices), but is otherwise straightforward. Many software programs provide solutions to systems of linear equations, but for Case 2 and a large number of faces, a dedicated Gauss–Seidel algorithm can take advantage of the sparseness of the matrix. Consider for example a data set collected on $N=200$ faces. The size of matrix $\mathbf{U}$ is then $205\times205=42{,}025$ $(=N^2+10N+25)$ elements, of which 39,800 $(=N^2-N)$ are zero: a dedicated routine has to deal with only 2225 $(=11N+25)$ elements.

In a companion paper, Launeau and Robin (in preparation) illustrate and discuss several issues associated with the determination of ellipsoids from sectional fabric data, using Ellipsoid, a Visual Basic program that implements the method demonstrated here.

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Appendix A. Squared Frobenius norm of the error matrix $\mathbf{X}^I$

Since the error matrix, $\mathbf{X}^I$, is symmetric, its squared Frobenius norm can be re-written as:

$$F^I=(\chi^I_{22})^2+2(\chi^I_{23})^2+(\chi^I_{33})^2=Tr\left(\mathbf{X}^I\mathbf{X}^I\right) \quad \text{(A1)}$$

where Tr means the trace of $\mathbf{X}^I\mathbf{X}^I$ (see Goldberg, 1991, p. 333). It is convenient to switch to the summation convention on repeated subscripted indices, in which:

$$\chi^I_{ij}=b^I_{ij}-l^I_{il}l^I_{jm}b_{lm} \quad \text{(A2)}$$

where $i, j=2, 3$ and $l, m=1, 2, 3$. The squared Frobenius norm, i.e. the trace of the square of $\mathbf{X}^I$, is then:

$$F^I=l^I_{il}l^I_{in}l^I_{jm}l^I_{jo}b_{lm}b_{no}-2l^I_{il}l^I_{jm}b^I_{ij}b_{lm}+b^I_{ij}b^I_{ij} \quad \text{(A3)}$$

where $i, j=2, 3$ and $l, m, n, o=1, 2, 3$. This expression consists of three terms that we evaluate separately.

A.1. The first term: $l^I_{il}l^I_{in}l^I_{jm}l^I_{jo}b_{lm}b_{no}$

It is quadratic in the sought components of $\mathbf{B}$, and all its coefficients are only functions of the orientation of Face I. Orthogonality of the $\mathbf{L}^I$ matrix is expressed by:

$$l^I_{lm}l^I_{ln}=\delta_{mn} \quad \text{(A4)}$$

where $l, m, n=1, 2, 3$, and δ_{mn} is Kronecker's δ (also called the unit matrix).

However, because i and j are only cycled through two and three, orthogonality of $\mathbf{L}^I$ means that:

$$l^I_{il}l^I_{in}=\delta_{ln}-l^I_{1l}l^I_{1n}$$

and

$$l^I_{jm}l^I_{jo}=\delta_{mo}-l^I_{1m}l^I_{1o}$$

$$\begin{aligned}l^I_{il}l^I_{in}l^I_{jm}l^I_{jo}&=\left(\delta_{ln}-l^I_{1l}l^I_{1n}\right)\left(\delta_{mo}-l^I_{1m}l^I_{1o}\right)\\&=\delta_{ln}\delta_{mo}-\delta_{mo}l^I_{1l}l^I_{1n}-\delta_{ln}l^I_{1m}l^I_{1o}+l^I_{1l}l^I_{1m}l^I_{1n}l^I_{1o}\end{aligned}$$

We see that only the direction cosines of the normal to Face I remain. Since $\mathbf{B}$ is symmetric:

$$l^I_{il}l^I_{in}l^I_{jm}l^I_{jo}b_{lm}b_{no}=\left(\delta_{ln}\delta_{mo}-2\delta_{mo}l^I_{1l}l^I_{1n}+l^I_{1l}l^I_{1m}l^I_{1n}l^I_{1o}\right)b_{lm}b_{no}$$

or

$$l^I_{il}l^I_{in}l^I_{jm}l^I_{jo}b_{lm}b_{no} = b_{lm}b_{lm} - 2l^I_{1m}l^I_{1n}b_{lm}b_{ln} + l^I_{1l}l^I_{1m}l^I_{1n}l^I_{1o}b_{lm}b_{no} \tag{A5a}$$

Now:

$$b_{lm}b_{lm} = (b_{11})^2+(b_{22})^2+(b_{33})^2+2\left[(b_{23})^2+(b_{13})^2+(b_{12})^2\right]$$

$$l^I_{1m}l^I_{1n}b_{lm}b_{ln} = l^I_{1m}l^I_{1n}(b_{1m}b_{1n} + b_{2m}b_{2n} + b_{3m}b_{3n})$$

and the last expression stands for $3^4 = 81$ separate terms. With all the expressions put together, they can be written in matrix form so as to highlight the independent parameters:

$$l^I_{il}l^I_{in}l^I_{jm}l^I_{jo}b_{lm}b_{no} = \begin{bmatrix} b_{11} & b_{22} & b_{33} & b_{23} & b_{13} & b_{12} \end{bmatrix} \mathbf{R}^I \begin{bmatrix} b_{11} \\ b_{22} \\ b_{33} \\ b_{23} \\ b_{13} \\ b_{12} \end{bmatrix} \tag{A5b}$$

where:

$$\mathbf{R}^I = \begin{bmatrix}
\left[1-(l^I_{11})^2\right]^2 & (l^I_{11}l^I_{12})^2 & (l^I_{11}l^I_{13})^2 & 2(l^I_{11})^2 l^I_{12}l^I_{13} & -2\left[1-(l^I_{11})^2\right]l^I_{11}l^I_{13} & -2\left[1-(l^I_{11})^2\right]l^I_{11}l^I_{12} \\
(l^I_{11}l^I_{12})^2 & \left[1-(l^I_{12})^2\right]^2 & (l^I_{12}l^I_{13})^2 & -2\left[1-(l^I_{12})^2\right]l^I_{12}l^I_{13} & 2(l^I_{12})^2 l^I_{11}l^I_{13} & -2\left[1-(l^I_{12})^2\right]l^I_{11}l^I_{12} \\
(l^I_{11}l^I_{13})^2 & (l^I_{12}l^I_{13})^2 & \left[1-(l^I_{13})^2\right]^2 & -2\left[1-(l^I_{13})^2\right]l^I_{12}l^I_{13} & -2\left[1-(l^I_{13})^2\right]l^I_{11}l^I_{13} & 2(l^I_{13})^2 l^I_{11}l^I_{12} \\
2(l^I_{11})^2 l^I_{12}l^I_{13} & -2\left[1-(l^I_{12})^2\right]l^I_{12}l^I_{13} & -2\left[1-(l^I_{13})^2\right]l^I_{12}l^I_{13} & 2\left[(l^I_{11})^2+2(l^I_{12}l^I_{13})^2\right] & 2l^I_{11}l^I_{12}\left[2(l^I_{13})^2-1\right] & 2l^I_{11}l^I_{13}\left[2(l^I_{12})^2-1\right] \\
-2\left[1-(l^I_{11})^2\right]l^I_{11}l^I_{13} & 2(l^I_{12})^2 l^I_{11}l^I_{13} & -2\left[1-(l^I_{13})^2\right]l^I_{11}l^I_{13} & 2l^I_{11}l^I_{12}\left[2(l^I_{13})^2-1\right] & 2\left[(l^I_{12})^2+2(l^I_{11}l^I_{13})^2\right] & 2l^I_{12}l^I_{13}\left[2(l^I_{11})^2-1\right] \\
-2\left[1-(l^I_{11})^2\right]l^I_{11}l^I_{12} & -2\left[1-(l^I_{12})^2\right]l^I_{11}l^I_{12} & 2(l^I_{13})^2 l^I_{11}l^I_{12} & 2l^I_{11}l^I_{13}\left[2(l^I_{12})^2-1\right] & 2l^I_{12}l^I_{13}\left[2(l^I_{11})^2-1\right] & 2\left[(l^I_{13})^2+2(l^I_{11}l^I_{12})^2\right]
\end{bmatrix}$$

A.1.1. Properties of $\mathbf{R}^I$

The necessary but confusing presence of superscripts, subscripts and exponents hides the fact that all components of $\mathbf{R}^I$ are functions of only three parameters: l^I_{11}, l^I_{12} and l^I_{13}; they are the direction cosines of the direction normal to Face *I*. In fact, all components are either quadratic or biquadratic in the direction cosines: therefore, the sense of the normal does not affect the result. In other words, it does not matter whether one uses a right-handed or left-handed coordinate system to describe Face *I*.

A.1.1.1. Rank of $\mathbf{R}^I$

Since it is a real symmetric matrix, we know that its eigenvalues must be real. Inspection of its components reveals that, if those in the first column are all multiplied by $(l^I_{11})^2$, those in the fifth column by $\frac{1}{2}l^I_{11}l^I_{13}$, and those in the sixth column by $\frac{1}{2}l^I_{11}l^I_{12}$, then the sum of these three terms is zero for all rows. Symbolically, we can write this as:

$$\left(l^I_{11}\right)^2\times[\text{Col. 1}] + \tfrac{1}{2}l^I_{11}l^I_{13}[\text{Col. 5}] + \tfrac{1}{2}l^I_{11}l^I_{12}[\text{Col. 6}] = [0]$$

Similarly,

$$\left(l^I_{12}\right)^2\times[\text{Col. 2}] + \tfrac{1}{2}l^I_{11}l^I_{12}[\text{Col. 6}] + \tfrac{1}{2}l^I_{12}l^I_{13}[\text{Col. 4}] = [0]$$

$$\left(l^I_{13}\right)^2\times[\text{Col. 3}] + \tfrac{1}{2}l^I_{12}l^I_{13}[\text{Col. 4}] + \tfrac{1}{2}l^I_{11}l^I_{13}[\text{Col. 5}] = [0]$$

In other words, there are three homogeneous linear relations among columns of $\mathbf{R}^I$. The rank of $\mathbf{R}^I$ is therefore only three. Stated differently, this means that three of its eigenvalues are zero. The significance of this is that $\mathbf{R}^I$ cannot be inverted. In other words, as we already know, one cannot determine the ellipsoid from one section only.

Since the Frobenius norm, by its very definition, must be $\geqq 0$, for any value of the components of $\mathbf{B}$, we conclude that $\mathbf{R}^I$ is positive semi-definite (e.g. Goldberg, 1991, pp. 365 and ff). This means that its non-zero eigenvalues are positive.

A.2. The second term: $l^I_{il}l^I_{jm}b^I_{ij}b_{lm}$

This term is linear in both the measured parameters and in the unknown components of $\mathbf{B}$ sought. We may represent it as the matrix product:

$$b_{lm}l^I_{il}l^I_{jm}b^I_{ij} = \begin{bmatrix} b_{11} & b_{22} & b_{33} & b_{23} & b_{13} & b_{12} \end{bmatrix} \times \begin{bmatrix} l^I_{21}l^I_{21} & l^I_{21}l^I_{31} & l^I_{31}l^I_{31} \\ l^I_{22}l^I_{22} & l^I_{22}l^I_{32} & l^I_{32}l^I_{32} \\ l^I_{23}l^I_{23} & l^I_{23}l^I_{33} & l^I_{33}l^I_{33} \\ 2l^I_{22}l^I_{23} & l^I_{22}l^I_{33} + l^I_{23}l^I_{32} & 2l^I_{32}l^I_{33} \\ 2l^I_{21}l^I_{23} & l^I_{21}l^I_{33} + l^I_{23}l^I_{31} & 2l^I_{31}l^I_{33} \\ 2l^I_{21}l^I_{22} & l^I_{21}l^I_{32} + l^I_{22}l^I_{31} & 2l^I_{31}l^I_{32} \end{bmatrix} \begin{bmatrix} b^I_{22} \\ 2b^I_{23} \\ b^I_{33} \end{bmatrix} \tag{A6a}$$

or

$$b_{lm}l^I_{il}l^I_{jm}b^I_{ij} = \begin{bmatrix} b_{11} & b_{22} & b_{33} & b_{23} & b_{13} & b_{12} \end{bmatrix} \mathbf{S}^I \tag{A6b}$$

in which $\mathbf{S}^I$ is a column matrix, of components $S^I_1, S^I_2, \ldots, S^I_6$.

A.3. The third term: $b^I_{ij}b^I_{ij}$

The third polynomial is a function only of the measured parameters, b^I_{22}, b^I_{23}, and b^I_{33}, on Face *I*. Its one component is, in fact, the squared Frobenius norm of the matrix representing the sectional ellipse:

$$\left|\mathbf{T}^I\right| = b^I_{ij}b^I_{ij} = \left(b^I_{22}\right)^2 + 2\left(b^I_{23}\right)^2 + \left(b^I_{33}\right)^2 \tag{A7}$$

Appendix B. Rewriting squared Frobenius norms for the unknown f^I (Case 2)

B.1. Squared Frobenius norm for a single face

When the measured parameters of the sectional ellipse on Face *I* consist only of an axial ratio and an angle, it is useful to rewrite the squared norm to make the additional unknown, f^I, explicit. Since coefficients of $\mathbf{R}^I$ are only functions of the orientation of Face *I*, not of the measured ellipse parameters, they are not affected by the change.

Inserting Eq. (10) into Eqs. (A6) and (A7), we find that $\mathbf{S}^I$ and $\mathbf{T}^I$ become respectively:

$$\mathbf{S}^I = f^I \begin{bmatrix} l^I_{21}l^I_{21} & l^I_{21}l^I_{31} & l^I_{31}l^I_{31} \\ l^I_{22}l^I_{22} & l^I_{22}l^I_{32} & l^I_{32}l^I_{32} \\ l^I_{23}l^I_{23} & l^I_{23}l^I_{33} & l^I_{33}l^I_{33} \\ 2l^I_{22}l^I_{23} & 2l^I_{22}l^I_{33} & 2l^I_{32}l^I_{33} \\ 2l^I_{21}l^I_{23} & 2l^I_{21}l^I_{32} & 2l^I_{31}l^I_{33} \\ 2l^I_{21}l^I_{22} & 2l^I_{21}l^I_{32} & 2l^I_{31}l^I_{32} \end{bmatrix} \begin{bmatrix} \hat{b}^I_{22} \\ 2\hat{b}^I_{23} \\ \hat{b}^I_{33} \end{bmatrix} = \hat{\mathbf{S}}^I f^I \tag{B1}$$

$$T^I = \left|\mathbf{T}^I\right| = \left(f^I\right)^2 \left\{ \left(\hat{b}^I_{22}\right)^2 + 2\left(\hat{b}^I_{23}\right)^2 + \left(\hat{b}^I_{33}\right)^2 \right\} = \hat{T}^I \left(f^I\right)^2 \tag{B2}$$

Note that if the two parameters measured on Face *I* are ratio ρ^I and angle α^I:

$$\hat{T}^I = \left(\rho^I\right)^2 + \frac{1}{\left(\rho^I\right)^2} \tag{B3}$$

The squared norm can be rewritten:

$$F^I = \begin{bmatrix} b_{11} & b_{22} & b_{33} & b_{23} & b_{13} & b_{12} \end{bmatrix} \times \left\{ \mathbf{R}^I \begin{bmatrix} b_{11} \\ b_{22} \\ b_{33} \\ b_{23} \\ b_{13} \\ b_{12} \end{bmatrix} - 2\hat{\mathbf{S}}^I f^I \right\} + \hat{\mathbf{T}}^I \left(f^I\right)^2 \tag{B4}$$

We note that it is a homogeneous quadratic expression of the six components of $\mathbf{B}$ and of the scale parameter f^I. Components of $\mathbf{R}^I$ are the same as in Appendix A, i.e. still only functions of the orientation of the normal to Face *I*. Components of $\hat{\mathbf{S}}^I$ are mixed functions of the direction cosines of the axes in Face *I* and of the measured parameters. And $\hat{T}^I$ is a Frobenius norm of the measured sectional ellipse, which is only a function of the measured axial ratio (Eq. (B3)).

B.2. 'Squared Frobenius sum'

If we add the squared norms for *N* faces, their sum is:

$$F = \begin{bmatrix} b_{11} & b_{22} & b_{33} & b_{23} & b_{13} & b_{12} \end{bmatrix} \times \left\{ \mathbf{R} \begin{bmatrix} b_{11} \\ b_{22} \\ b_{33} \\ b_{23} \\ b_{13} \\ b_{12} \end{bmatrix} - 2 \begin{bmatrix} \hat{S}^1_1 & \hat{S}^2_1 & \hat{S}^3_1 & \cdots & \hat{S}^N_1 \\ \hat{S}^1_2 & \hat{S}^2_2 & \hat{S}^3_2 & \cdots & \hat{S}^N_2 \\ \hat{S}^1_3 & \hat{S}^2_3 & \hat{S}^3_3 & \cdots & \hat{S}^N_3 \\ \hat{S}^1_4 & \hat{S}^2_4 & \hat{S}^3_4 & \cdots & \hat{S}^N_4 \\ \hat{S}^1_5 & \hat{S}^2_5 & \hat{S}^3_5 & \cdots & \hat{S}^N_5 \\ \hat{S}^1_6 & \hat{S}^2_6 & \hat{S}^3_6 & \cdots & \hat{S}^N_6 \end{bmatrix} \begin{bmatrix} f^1 \\ f^2 \\ f^3 \\ \vdots \\ f^N \end{bmatrix} \right\} + \begin{bmatrix} \hat{T}^1 & 0 & 0 & \cdots & 0 \\ 0 & \hat{T}^2 & 0 & \cdots & 0 \\ 0 & 0 & \hat{T}^3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & 0 & \hat{T}^N \end{bmatrix} \begin{bmatrix} f^1 \\ f^2 \\ f^3 \\ \vdots \\ f^N \end{bmatrix} \tag{B5}$$

In order to bring out better the homogeneous quadratic form of the expression, it can be re-written as a single matrix product (Eq. (23)). It is convenient for what follows to call $\mathbf{U}$ the $(N+6) \times (N+6)$ real symmetric matrix in Eq. (23).

We see that F is a homogeneous quadratic function of all the unknowns. From the very definition of F as a sum of norms that can each only be positive or zero, we know that F itself can only be positive or zero. The quadratic form is thus said to be either *positive definite*, in which case all eigenvalues of $\mathbf{U}$ are positive, or *positive semi-definite*, in which case one or more eigenvalue(s) of $\mathbf{U}$ may be zero (e.g. Goldberg, 1991, pp. 365 and ff). In general, if three or more different directions contribute to it, all eigenvalues of $\mathbf{U}$ are positive, its rank is $N+6$, and the form is positive definite. However, if artificial data are generated such that compatibility between them is perfect, one eigenvalue is equal to zero, and the form is positive semi-definite. The best-fit solution (see Appendix C) is then given by the corresponding eigenvector, i.e. by the linear combination of the parameters for which indeed $F=0$.

Appendix C. Finding the constrained minimum of F for Case 2

By substituting $(3-b_{22}-b_{33})$ for b_{11} into Eq. (23), it can be rewritten as shown in (C1):

$$F=\begin{bmatrix} b_{22} & b_{33} & b_{23} & b_{13} & b_{12} & f^1 & \cdots & f^N \end{bmatrix} \times\left\{\mathbf{U}'\begin{bmatrix} b_{22}\\ b_{33}\\ b_{23}\\ b_{13}\\ b_{12}\\ f^1\\ \vdots\\ f^N \end{bmatrix}+6\begin{bmatrix} R_{12}-R_{11}\\ R_{13}-R_{11}\\ R_{14}\\ R_{15}\\ R_{16}\\ -\hat{S}_1^1\\ \vdots\\ -\hat{S}_1^N \end{bmatrix}\right\}+9R_{11} \qquad \text{(C1)}$$

where $\mathbf{U}'$ is a symmetric $(N+5)\times(N+5)$ matrix obtained from $\mathbf{U}$ by subtracting its line 1 from its lines 2 and 3, subtracting its column 1 from its columns 2 and 3, and eliminating line 1 and column 1. The minimum of F corresponds to the solution of the system of $(N+5)$ linear equations in $(N+5)$ unknowns obtained by equating to zero all derivatives of F with respect to $b_{22}, b_{33}, \ldots, f^1, \ldots, f^N$. Introducing the weights, w^I, which quantify our relative confidence in each section I (Section 6), the system of equations to be solved, written in matrix form, is (C2):

$$\begin{bmatrix}
R_{22}-2R_{12} & R_{23}-R_{12}-R_{13} & R_{24}-R_{14} & R_{25}-R_{15} & R_{26}-R_{16} & w^1\left(\hat{S}_1^1-\hat{S}_2^1\right) & w^2\left(\hat{S}_1^2-\hat{S}_2^2\right) & \cdots & w^N\left(\hat{S}_1^N-\hat{S}_2^N\right)\\
R_{23}-R_{12}-R_{13} & R_{33}-2R_{13} & R_{34}-R_{14} & R_{35}-R_{15} & R_{36}-R_{16} & w^1\left(\hat{S}_1^1-\hat{S}_3^1\right) & w^2\left(\hat{S}_1^2-\hat{S}_3^2\right) & \cdots & w^N\left(\hat{S}_1^N-\hat{S}_3^N\right)\\
R_{24}-R_{14} & R_{34}-R_{14} & R_{44} & R_{45} & R_{46} & -w^1\hat{S}_4^1 & -w^2\hat{S}_4^2 & \cdots & -w^N\hat{S}_4^N\\
R_{25}-R_{15} & R_{35}-R_{15} & R_{45} & R_{55} & R_{56} & -w^1\hat{S}_5^1 & -w^2\hat{S}_5^2 & \cdots & -w^N\hat{S}_5^N\\
R_{26}-R_{16} & R_{36}-R_{16} & R_{46} & R_{56} & R_{66} & -w^1\hat{S}_6^1 & -w^2\hat{S}_6^2 & \cdots & -w^N\hat{S}_6^N\\
\hat{S}_1^1-\hat{S}_2^1 & \hat{S}_1^1-\hat{S}_3^1 & -\hat{S}_4^1 & -\hat{S}_5^1 & -\hat{S}_6^1 & \hat{T}^1 & 0 & \cdots & 0\\
\hat{S}_1^2-\hat{S}_2^2 & \hat{S}_1^2-\hat{S}_3^2 & -\hat{S}_4^2 & -\hat{S}_5^2 & -\hat{S}_6^2 & 0 & \hat{T}^2 & \cdots & 0\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & 0\\
\hat{S}_1^N-\hat{S}_2^N & \hat{S}_1^N-\hat{S}_3^N & -\hat{S}_4^N & -\hat{S}_5^N & -\hat{S}_6^N & 0 & 0 & 0 & \hat{T}^N
\end{bmatrix}
\times\begin{bmatrix} b_{22}\\ b_{33}\\ b_{23}\\ b_{13}\\ b_{12}\\ f^1\\ f^2\\ \vdots\\ f^N \end{bmatrix}=-3\begin{bmatrix} R_{12}-R_{11}\\ R_{13}-R_{11}\\ R_{14}\\ R_{15}\\ R_{16}\\ -\hat{S}_1^1\\ -\hat{S}_1^2\\ \vdots\\ -\hat{S}_1^N \end{bmatrix} \qquad \text{(C2)}$$

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