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EXCALIBR II

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Dedicated to Emeritus Professor Hans Wondratschek
on his retirement from active duty, but not from active research

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Abstract. The computer program EXCALIBR (Bloss and Riess, 1973; Bloss, 1981, p. 202) has been rewritten and markedly improved. Like EXCALIBR, EXCALIBR II solves optical extinction data, as determined with a spindle stage, and determines the optic axial angle 2V and the orientation of the crystal's optical indicatrix. EXCALIBR II uses a modification to Joel's equation as a means of obtaining the optic axes of a crystal. The new algorithm eliminates the need to solve the extinction data, quartet by quartet, as the first step towards finding a solution, as required by EXCALIBR. Furthermore, EXCALIBR II successfully solves extinction data where one optic axis of a biaxial crystal is 90° to the spindle axis, an orientation that had thwarted its predecessor. EXCALIBR II also accurately determines the optical indicatrix orientation for uniaxial crystals. The new program runs 10 times faster than EXCALIBR. In addition, creating data files is simplified by free-formatted input.

After solving extinction data for several different wavelengths and/or temperatures, EXCALIBR II calculates the angular change of each optic direction with wavelength and/or temperature along with the error on the angle. Using a simple t-test, it then computes a p-value to aid in the decision as to whether the optical direction truly exhibits dispersion. This is a more valid and sensitive procedure than the χ^2 test used by EXCALIBR, particularly because the covariance in each optic vector's coefficients are taken into consideration and the results are invariant to the vector's orientation.

Introduction

Optical properties are a fundamental physical property of a mineral. Since its development in 1959, the spindle stage method for determining the refractive indices of crystals has led to a significant improvement in the measurement of optical data (Wilcox, 1959; Bloss, 1978; Bloss, 1981). Basically, the method involves first mounting a crystal on the needle tip of a spindle stage. Next, the spindle stage is mounted on the stage of a polarizing microscope where the crystal is submerged in an immersion oil. Using polarized monochromatic light, the crystal is then systematically rotated around the spindle axis and around the microscope axis until the crystal becomes extinct. These two degrees of rotation plus an analysis of a wide range of extinction positions permit the determination of the orientation of the optical indicatrix (Bloss and Riess, 1973; Bloss, 1981, p. 63).

The program EXCALIBR was developed to computationally analyze these extinction data and determine the coordinates of a biaxial optical indicatrix (Bloss and Riess, 1973; Bloss, 1981, p. 202). These coordinates, in turn, indicate the precise orientation at which to measure the crystal's principle refractive indices α, β and γ. The combination of spindle stage methods and EXCALIBR has been used to solve and discover numerous problems in optical mineralogy (Armbruster and Bloss, 1982; Gunter and Bloss, 1982; Su et al., 1984; Greiner and Bloss, 1987). However, the computational procedure used by EXCALIBR placed various restrictions on both extinction data accuracy and crystal orientation (Bloss and Riess, 1973; Bloss, 1981, p. 217). In addition, there were problems with the estimated standard deviations of the coordinates and the statistical methods used for dispersion analysis (Bloss, 1981, p. 308).

Consequently, a new version of EXCALIBR has been written by two of us (K. L. B. and R. T. D.) in collaboration with the others (F. D. B. and J. B. B.). Like EXCALIBR, the new program temporarily called EXCALIBR II, but eventually to assume the name of its predecessor, uses the equation

$$(\mathbf{q} \cdot \mathbf{a}_1)(\mathbf{q} \cdot \mathbf{a}_2) - (\mathbf{p} \cdot \mathbf{a}_1)(\mathbf{p} \cdot \mathbf{a}_2) = 0 \qquad (1)$$

introduced by Joel (Joel, 1965) in determining estimates ($^\wedge$) for the two normalized optic axes, $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$. This algorithm, as used by EXCALIBR, solves for six variables subject to the constraint that the two optic axes are normalized (Bloss and Riess, 1973). Using six variables leads to an ill-conditioned problem that requires accurate starting estimates. This was accomplished by organizing the data into groups of four whose spindle axis settings (S values) differed by at least 40°. For each group, EXCALIBR determines estimates for $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ and uses their average as starting values for the least-squares problem (Bloss and Riess, 1973). The new algorithm (described below) used by EXCALIBR II only involves four variables which has significantly improved the conditioning of the problem. As a consequence, the new program eliminates the need to organize the data into groups. This constitutes a major advantage. Now, even if optical extinctions can only be measured over a limited range of spindle settings, the optic axial angle 2V and the orientation of the indicatrix can be determined. In addition, the number of lines of code involved are about two thirds the original number and the run-time is reduced. EXCALIBR's computation time, operating at 10 megahertz for the Tiburon albite data (presented as an example), was approximately 1 minute, 37 seconds; EXCALIBR II's was 10 seconds. EXCALIBR II thus provides an approximate 90% reduction in computation time. The physical storage space required for EXCALIBR II has also been reduced by 40% to approximately 1 K. In addition, data input has been significantly simplified over that of EXCALIBR primarily because of free format input.

Copies of EXCALIBR II may be obtained by sending a check for $20.00 made out to the Virginia Tech Foundation – Geology Fund, along with the disk type specification to K. L. B. or R. T. D. The source code, executable file, example data, and input instructions will be included on a returned disk. The source code is written in double precision standard Fortran 77 and should compile on any operating system. The program can be copied and distributed freely.

Program procedure

A complete description of the data input is provided with the program. An example input data file, for the Tiburon albite discussed in the paper, is shown in Figure 1 to illustrate the simplicity of the input data structure. In general, the input file contains the spindle setting, S, followed by the microscope stage settings, M_s, that provided crystal extinction. Note that input of the reference azimuth, M_r, is now optional. M_r is the microscope stage setting that aligns the spindle axis precisely east-west (Bloss, 1981, p. 19).

Provided no M_r value was input, EXCALIBR II first calculates the average reference azimuth, $\overline{M}_r$, from all supplied M_s data whose S values differ by 180°. For example, if extinction data are supplied for S values from 0°, 10°,..., 350°, as in the so-called 360° option of EXCALIBR, EXCALIBR II calculates M_r for each of the 18 pairs of data. It then uses $\overline{M}_r$, the average of these 18 values of M_r in its calculations.

Next, the program uses the input M_r or the computed $\overline{M}_r$ to calculate, for all S settings, a corrected extinction angle E_s, where

$$E_s = M_s - \overline{M}_r.$$

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* * * top of file * * *
Tiburon Albite - Wolfe
433 500 600 666/
/
0      217.9 218   218.1 218.2
10     218.5 218.3 218.3 218.6
20     219.1 219.3 219.2 219.5
30     219.6 219.7 219.5 219.3
40     219.4 219.6 219.3 219.2
50     218.6 218.6 218.9 219
60     217.3 217.3 216.8 216.9
70     213.6 213.6 213.8 213.7
80     205.9 205.9 206.4 206.4
90     189.9 189.9 191.3 191.6
100    171.7 171.7 172.8 172.5
110    159.2 159.2 159.5 159.8
120    153   153   153.6 154
130    149.8 149.8 149.7 150.4
140    147.1 147.4 147.7 147.8
150    145.8 145.7 145.9 146.1
160    144.4 144.6 144.6 144.5
170    143.5 143.4 143.4 143.5
180    142.4 142.3 142.2 142.1
* * * end of file * * *
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Fig. 1. Example input data file showing extinction data for the Tiburon Albite measured at wavelengths of 433, 500, 600 and 666 nm (Bloss, 1981, p. 210). A line by line description of the input data file is provided with the program.

Two equivibration directions **p** and **q** are then calculated by adding and subtracting 45° from each E_s angle, respectively. The angular coordinates for **p** and **q** are then converted to a Cartesian coordinate system ($C = \{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$) defined relative to the microscope where $[\mathbf{p}]^t_C = [p_1\, p_2\, p_3]$ and $[\mathbf{q}]^t_C = [q_1\, q_2\, q_3]$. The x-axis is defined to be east-west, the y-axis north-south, and the z-axis is defined to be perpendicular to the microscope stage.

After rewriting Joel's equation (Equation 1) in term of four variables, a, b, c and d,

$$\begin{aligned}[(q_1q_2 - p_1p_2) + (q_2^2 - p_2^2)c + (q_2q_3 - p_2p_3)d]a \\ + [(q_1q_3 - p_1p_3) + (q_3^2 - p_3^2)d + (q_2q_3 - p_2p_3)c]b \\ + [(q_1q_2 - p_1p_2)]c + [(q_1q_3 - p_1p_3)]d \\ = -(q_1^2 - p_1^2)\,,\end{aligned}$$

the program employs the Gauss-Newton algorithm (GN) (Seber and Wild, 1989) to obtain unbiased, minimum variance estimates: $\hat{a} = \hat{s}/\hat{r}$, $\hat{b} = \hat{t}/\hat{r}$, $\hat{c} = \hat{v}/\hat{u}$ and $\hat{d} = \hat{w}/\hat{u}$. The program is considered to converge when the parameter shifts, $\Delta\hat{a}$, $\Delta\hat{b}$, $\Delta\hat{c}$ and $\Delta\hat{d}$, are less than 1.0×10^{-14}. Estimated final coordinates for $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$, where $[\hat{\mathbf{a}}_1]^t_C = [\hat{r}\,\hat{s}\,\hat{t}]$ and $[\hat{\mathbf{a}}_2]^t_C = [\hat{u}\,\hat{v}\,\hat{w}]$, are obtained from the normalization condition. Given the optic axes, computation of estimates for the acute and obtuse bisectrix and the optic normal vectors is obtained by adding, subtracting, and forming the cross product, respectively.

In the case where the program is unable to converge to a set of parameter estimates after 100 iterations, it is likely that one of the optic axes is located in the yz plane, in other words, 90° from the spindle axis. This will cause the estimates of the regression parameters to increase to infinity since either $\hat{r}$ or $\hat{u}$ would equal zero. To obviate this difficulty, all **p** and **q** data are rotated 120° about the vector $[111]_C^t$. If convergence is again not achieved after 100 iterations (implying that $\hat{s}$ or $\hat{v}$ equal zero), then the optic axis must coincide with the z-axis, that is, it is located in xz *and* yz planes. This requires all **p** and **q** data to be rotated another 120° about the vector $[111]_C^t$. Once convergence has been reached, the estimated optic axes are then transformed back to the original orientation.

Estimates for a single optic axis, ε, (uniaxial crystals) where $[\hat{\varepsilon}]_C^t = [\hat{e}\,\hat{f}\,\hat{g}]$, are determined by rewriting Joel's Equation (Equation 1) in the following form

$$[2(q_1q_2 - p_1p_2) + (q_2^2 - p_2^2)a + (q_2q_3 - p_2p_3)b]a$$
$$+ [2(q_1q_3 - p_1p_3) + (q_3^2 - p_3^2)b + (q_2q_3 - p_2p_3)a]b = -(q_1^2 - p_1^2)\ .$$

Minimum variance estimates of a and b using the GN method (Seber and Wild, 1989) are computed where $\hat{a} = \hat{f}/\hat{e}$, $\hat{b} = \hat{g}/\hat{e}$. The program is considered to converge when the parameter shifts, $\Delta\hat{a}$ and $\Delta\hat{b}$ are less than 1.0×10^{-14}. Final coordinates for $\hat{\varepsilon}$ are again obtained from the normalization condition.

An estimate of the covariance matrix, V_s, for the optic axes is obtained from the propagation of error equation (Kendal and Stuart, 1987)

$$\hat{V}_s = L^t \hat{V}_m L \tag{2}$$

where $\hat{V}_m$ is the estimated covariance matrix of the four (or two) estimated regression parameters (Milton and Arnold, 1990) and L^t is the transpose of the matrix L:

$$L = \begin{bmatrix} \partial r/\partial a & \partial s/\partial a & \partial t/\partial a & \partial u/\partial a & \partial v/\partial a & \partial w/\partial a \\ \partial r/\partial b & \partial s/\partial b & \partial t/\partial b & \partial u/\partial b & \partial v/\partial b & \partial w/\partial b \\ \partial r/\partial c & \partial s/\partial c & \partial t/\partial c & \partial u/\partial c & \partial v/\partial c & \partial w/\partial c \\ \partial r/\partial d & \partial s/\partial d & \partial t/\partial d & \partial u/\partial d & \partial v/\partial d & \partial w/\partial d \end{bmatrix} .$$

The estimated standard errors, given in the output for $\hat{r}$, $\hat{s}$, $\hat{t}$, and $\hat{u}$, $\hat{v}$, $\hat{w}$ are the square roots of the diagonal elements of $\hat{V}_s$, respectively. Similarly,

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Tiburon Albite - Wolfe

 Experimental Treatment ID number  =    433.000
 Average Reference Azimuth, Mr (esd) =  180.15 (   .00)
 based on   4 observations.

 Biaxial Model
 number of iterations(100 max.) =    7
 R-squared =    .99956
 m.s.e.  =   .000425

        S          Ms          Es       CALC(Es)   Es-CALC(Es)
       .00      217.90       37.75       37.74        .01
     10.00      218.50       38.35       38.49       -.14
     20.00      219.10       38.95       39.04       -.09
     30.00      219.60       39.45       39.31        .14
     40.00      219.40       39.25       39.19        .06
     50.00      218.60       38.45       38.50       -.05
     60.00      217.30       37.15       36.85        .30
     70.00      213.60       33.45       33.39        .06
     80.00      205.90       25.75       26.01       -.26
     90.00      189.90        9.75       10.56       -.81
    100.00      171.70      171.55      170.77        .78
    110.00      159.20      159.05      158.86        .19
    120.00      153.00      152.85      152.93       -.08
    130.00      149.80      149.65      149.55        .10
    140.00      147.10      146.95      147.31       -.36
    150.00      145.80      145.65      145.65        .00
    160.00      144.40      144.25      144.31       -.06
    170.00      143.50      143.35      143.20        .15
    180.00      142.40      142.25      142.26       -.01

 Optic Axial Angle, 2V (ese) =  77.567 ( .368)

  Computed Cartesian Coordinates
              x      (ese)              y      (ese)            z      (ese)
 OA1        .9875 ( .0006)         -.0205 ( .0038)          .1565 ( .0040)
 OA2        .2304 ( .0027)          .9719 ( .0007)          .0494 ( .0035)
 AB         .7811 ( .0006)          .6102 ( .0008)          .1321 ( .0019)
 OB         .6044 ( .0010)         -.7921 ( .0006)          .0855 ( .0055)
 ON       -.1568 ( .0039)          -.0131 ( .0043)          .9875 ( .0006)

  Spindle Stage Coordinates to measure refractive indices.
              S     (ese)          Es     (ese)                 Ms
 OA1        97.45 ( 1.40)         9.08 (   .23)
 OA2         2.91 (   .21)       76.68 (   .16)     (e-w polr.)   (n-s polr.)
 AB         12.21 (   .17)       38.64 (   .06)       218.79        128.79
 OB        173.84 (   .39)       52.82 (   .07)       232.97        142.97
 ON         90.76 (   .25)       99.02 (   .23)       279.17        189.17
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Fig. 2. Select portion of EXCALIBR II output file showing solution of the 433 nm data provided in Figure 1. For comparison with EXCALIBR, see Bloss (1981, p. 210).

estimated standard errors of other quantities are obtained by propagation of error from $\hat{V}_s$.

Bloss (1981, p. 210) presents EXCALIBR's solutions of extinction data determined at wavelengths 433, 500, 600 and 666 nm for an albite from

Tiburon, California. The solutions for all wavelengths closely compare to the new solutions determined for the data by EXCALIBR II. For comparison Figure 2 shows the results for EXCALIBR II's 433 nm solution. The most significant differences occur in calculations of the estimated standard errors. Those calculated by EXCALIBR II are slightly larger than those calculated by EXCALIBR. It has been suspected that the estimated standard errors provided by EXCALIBR were too small (Bloss, 1981, p. 308).

Combined optical and X-ray studies

Following the determination of all solutions, the program calculates the upper and lower arc settings for the goniometer that will align a given optic vector along either the spindle axis (x-axis) or the light axis (z-axis). Arc settings are provided for both Type I and Type II goniometer heads (Bloss, 1981, p. 233). Of course not all arc settings will be attainable because of the limited rotation range of most goniometer arcs. If an optic direction that coincides with a crystallographic axis can be brought parallel to x, the crystal becomes oriented for a Weissenberg, oscillation, or rotation photograph. If it can be brought parallel to z, the crystal will be oriented for a precession photograph with the optic direction as the precessing axis. For triclinic crystals, a spindle stage study will not help orient the crystal for an X-ray photograph unless the angles between the optic vectors and the crystallographic axes are, at least, approximately known.

When a spindle stage study is followed by an X-ray study of the crystal, EXCALIBR II uses the before and after goniometer arc settings to calculate the coordinates that the optic vectors assume after the goniometer arcs were re-set for the X-ray study. This is accomplished by computing a transformation matrix

$$T = M_C({}^{[010]}\varrho_L)M_C({}^{[001]}\varrho_U)$$

where M_C represents a general Cartesian rotation matrix (Boisen and Gibbs, 1985) and ϱ_L and ϱ_U are the turn angles about the y- and z-axes, respectively. These new optic vector coordinates permit the user to continue the optical study at the current goniometer arc settings. In addition, these new coordinates permit the calculation of the precise angles between the estimated optical vectors and the estimated crystallographic axes determined from the X-ray study.

Statistical study of optical dispersion

Even with a simple detent spindle stage, the dispersion of the optical vectors or their change with temperature may be determined for a crystal. One simply needs to make careful spindle stage studies at two or more different conditions such as wavelengths or temperatures. For example, the wavelengths for which extinction positions were measured for the Tiburon albite sample are entered on line 2 (Fig. 1). Measurement of a crystal's optical dispersion can provide additional insight into structural features such as phase transitions or even possibly petrogenetic histories (Bloss, 1978). Statistics are necessary to help indicate whether the solutions determined for one treatment are really different from those solutions obtained from another treatment. By using a t-test to test the null hypothesis, H_0, of non-dispersion, EXCALIBR II provides an analysis of dispersion that is superior to that of its predecessor EXCALIBR.

When comparing two vectors, $\mathbf{v}_1$ and $\mathbf{v}_2$, for possible dispersion, the angle between the vectors, namely θ, is a natural parameter of interest. If θ equals zero, then obviously no dispersion occurred. However, because we can only estimate the optic vectors, $\hat{\mathbf{v}}_i$, we can only estimate the angle between vectors, $\hat{\theta}$. Thus, a finite estimated angle between estimated vectors does not necessarily indicate dispersion. Of equal importance is the estimated standard error of this angle, $\hat{\sigma}_{\hat{\theta}}$. Through propagation of error, EXCALIBR II computes a 3×3 estimated covariance matrix, $\hat{V}_{\hat{\mathbf{v}}_i}$, for the coordinates of each estimated optic vector $\hat{\mathbf{v}}_i$. By combining $\hat{V}_{\hat{\mathbf{v}}_i}$ for the two vectors under consideration, $\hat{\sigma}^2_{\hat{\theta}}$ is computed according to Equation 2 as

$$\hat{\sigma}^2_{\hat{\theta}} = L^t \begin{bmatrix} \hat{V}_{\hat{\mathbf{v}}_1} & \mathbf{O} \\ \mathbf{O} & \hat{V}_{\hat{\mathbf{v}}_2} \end{bmatrix} L \tag{3}$$

where

$$L = \begin{bmatrix} -\hat{x}_2/\sin\hat{\theta} \\ -\hat{y}_2/\sin\hat{\theta} \\ -\hat{z}_2/\sin\hat{\theta} \\ -\hat{x}_1/\sin\hat{\theta} \\ -\hat{y}_1/\sin\hat{\theta} \\ -\hat{z}_1/\sin\hat{\theta} \end{bmatrix},$$

$\mathbf{O}$ is a 3×3 matrix of zeros, $[\hat{\mathbf{v}}_1]^t_C = [\hat{x}_1\ \hat{y}_1\ \hat{z}_1]$, $[\hat{\mathbf{v}}_2]^t_C = [\hat{x}_2\ \hat{y}_2\ \hat{z}_2]$, and $\hat{\theta} = \cos^{-1}(\hat{x}_1\hat{x}_2 + \hat{y}_1\hat{y}_2 + \hat{z}_1\hat{z}_2)$.

EXCALIBR II uses the t-value ($t = \hat{\theta}/\hat{\sigma}_{\hat{\theta}}$) to determine a p-value from the appropriate t-distribution for the two vectors under consideration (Press et al., 1986). The p-value represents the probability of obtaining a statistic greater than or equal to the observed value, assuming the null hypothesis, $H_o : \theta = 0$, is true. Small p-values (≤ 0.10) suggest rejection of the null hypothesis of non-dispersion. In other words, small p-values imply dispersion.

An equally valid test for indicating statistical differences resulting from experimental treatments can be found by utilizing the estimated differences in coefficients of the compared vectors. If $\hat{\mathbf{v}}_1$ and $\hat{\mathbf{v}}_2$ are the vectors under consideration, then we define $\Delta\hat{\mathbf{v}}$ as

$$[\Delta\hat{\mathbf{v}}]_C = [\hat{\mathbf{v}}_1]_C - [\hat{\mathbf{v}}_2]_C = \begin{bmatrix} \Delta\hat{x} \\ \Delta\hat{y} \\ \Delta\hat{z} \end{bmatrix} = \begin{bmatrix} \hat{x}_1 - \hat{x}_2 \\ \hat{y}_1 - \hat{y}_2 \\ \hat{z}_1 - \hat{z}_2 \end{bmatrix}.$$

Multivariate theory suggests that a modified form of the Hotelling's T^2 statistic (Johnson and Wichern, 1982) be used to test the null hypothesis of nondispersion, $H_o : \Delta\mathbf{v} = 0$. The test statistic, T^2, is computed according to

$$T^2 = [\Delta\hat{\mathbf{v}}]_C^t \hat{S}_P^{-1} [\Delta\hat{\mathbf{v}}]_C \tag{4}$$

where $\hat{S}_P = (\hat{V}_{\hat{v}_1} + \hat{V}_{\hat{v}_2})/2$ is the pooled estimate of the covariance matrix for $\Delta\hat{\mathbf{v}}$. The null hypothesis is rejected if the p-value for T^2, determined from the appropriate F-distribution, is less than or equal to 0.10. As the number of observations or experimental measurements become very large ($N > 200$), then T^2 approximately follows a χ^2 distribution (Johnson and Wichern, 1982).

Assuming a χ^2 distribution with 2 degrees of freedom corresponding to the number of independent parameters, EXCALIBR used a χ^2-test statistic to test $H_0 : \Delta\mathbf{v} = 0$. Computationally, the χ^2-test statistic is analogous to T^2 given in Equation 4 except it assumes all off-diagonal covariance terms in $\hat{S}_P$ are zero, a situation often not true in practice. EXCALIBR's use of a χ^2-test statistic is inappropriate for several reasons. First the χ^2-test only follows a χ^2 distribution when the standard errors of compared parameters ($\sigma_{\Delta\hat{x}}$, $\sigma_{\Delta\hat{y}}$ and $\sigma_{\Delta\hat{z}}$) are known. In reality, however, these standard errors are unknown and we can only obtain estimates of them ($\hat{\sigma}_{\Delta\hat{x}}$, $\hat{\sigma}_{\Delta\hat{y}}$ and $\hat{\sigma}_{\Delta\hat{z}}$). Second, by using a χ^2-test statistic, EXCALIBR incorrectly ignored the inherent covariance between $\Delta\hat{x}$, $\Delta\hat{y}$ and $\Delta\hat{z}$. Recall that along with Joel's equation (Equation 1) are the constraints that $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ are normalized. Consequently, this constraint introduces correlation within the coefficients for each optic axis, and therefore because these coefficients are correlated, any vector computed using $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ must inherently have covariance between coefficients.

Ignoring the covariance between $\Delta\hat{x}$, $\Delta\hat{y}$ and $\Delta\hat{z}$ leads to a dependence of EXCALIBR's χ^2-test value on the orientation of $\Delta\hat{\mathbf{v}}$. EXCALIBR accounted for this orientation dependence essentially by rotating $\Delta\hat{\mathbf{v}}$ and computing a new χ^2-test. It then reported the harmonic mean of p-values determined from these various χ^2-test values (Bloss, 1981, p. 310). However like T^2, a true χ^2-test random variable (i.e. zero covariance) should have no orientation dependence.

Table 1. Comparison of dispersion analysis provided by EXCALIBR II and EXCALIBR. The dispersion analysis is computed for wavelengths between 433 and 666 nm. The analysis provided by EXCALIBR II is listed first and includes the angle between optic vectors (Ang) along with its estimated standard error (ese) and the p-value (p). The analysis provided by EXCALIBR is listed below.

Treatments		Optic axis 1			Optic axis 2			Acute bisectrix			Obtuse bisectrix			Optic normal		
		Ang	ese	p	Ang	ese	p	Ang	ese	p	Ang	ese	p	Ang	ese	p
433	500	0.327	0.347	0.354	0.144	0.297	0.632	0.114	0.153	0.464	0.356	0.479	0.462	0.369	0.471	0.439
		0.315	—	0.364	0.139	—	0.787	0.112	—	0.493	0.356	—	0.459	0.371	—	0.368
433	600	0.324	0.336	0.341	0.654	0.294	0.033	0.325	0.166	0.059	0.439	0.485	0.372	0.544	0.385	0.166
		0.205	—	0.744	0.626	—	0.002	0.337	—	0.004	0.434	—	0.265	0.541	—	0.016
433	666	0.948	0.352	0.011	0.852	0.275	0.004	0.522	0.168	0.004	0.055	0.331	0.870	0.522	0.178	0.006
		0.831	—	0.008	0.799	—	0.000	0.529	—	0.000	0.042	—	0.990	0.530	—	0.005
500	600	0.380	0.366	0.307	0.753	0.320	0.025	0.231	0.172	0.188	0.795	0.516	0.132	0.820	0.491	0.104
		0.343	—	0.258	0.740	—	0.000	0.243	—	0.069	0.789	—	0.015	0.814	—	0.001
500	666	0.735	0.369	0.054	0.895	0.304	0.006	0.415	0.180	0.027	0.320	0.538	0.555	0.525	0.333	0.124
		0.647	—	0.055	0.865	—	0.000	0.421	—	0.000	0.314	—	0.493	0.524	—	0.003
600	666	0.688	0.379	0.078	0.392	0.268	0.153	0.212	0.166	0.209	0.477	0.539	0.382	0.510	0.518	0.331
		0.673	—	0.020	0.382	—	0.067	0.212	—	0.027	0.476	—	0.244	0.510	—	0.126

To illustrate the invariance of T^2 on the orientation of $\Delta\hat{\mathbf{v}}$, let M_C represent a Cartesian rotation matrix, then according to Equation 4

$$T^2 = [\Delta\hat{\mathbf{v}}]_C^t \hat{S}_P^{-1} [\Delta\hat{\mathbf{v}}]_C = [\Delta\hat{\mathbf{v}}_r]_C^t \hat{S}_{P_r}^{-1} [\Delta\hat{\mathbf{v}}_r]_C, \quad (5)$$

where $M_C\Delta\hat{\mathbf{v}} = \Delta\hat{\mathbf{v}}_r$ and $\hat{S}_{P_r} = M_C\hat{S}_P M_C^{-1}$ is the estimated covariance matrix of $\Delta\hat{\mathbf{v}}_r$, the rotated vector. When computing the χ^2-test value, EXCALIBR uses only the diagonal elements of $\hat{S}_P^{-1}$. By recomputing the χ^2-test value for $\Delta\hat{\mathbf{v}}_r$ again using only the diagonal elements of $\hat{S}_{P_r}^{-1}$, the equality in Equation 5 is violated.

Our studies indicate that the simple t-test provides a better measure of dispersion than use of the Hotelling's T^2 for the current application. In addition, use of the t-value as a test statistic has several advantages over the χ^2-test statistic used by EXCALIBR. First of all, the t random variable directly employs the notion that we are only estimating the standard error, $\hat{\sigma}_{\hat{\theta}}$, of θ. The degrees of freedom used in the t-distribution now utilizes both the number of independent parameters under consideration and the number of experimental data used to compute $\hat{\theta}$. The degrees of freedom for the χ^2 distribution used by EXCALIBR was always two regardless of data size. Furthermore, the estimated covariance of the vector coefficients is incorporated into $\hat{\sigma}_{\hat{\theta}}$ according to Equation 3. In addition, the t random variable is independent of orientation because $\hat{\theta}$ and $\hat{\sigma}_{\hat{\theta}}$ is invariant under any rotation, M_C.

Table 1 shows the results of the dispersion analysis provided by both EXCALIBR and EXCALIBR II using the data from Figure 1. The probability values given by EXCALIBR have been converted to p-values for comparison with p-values from EXCALIBR II. By accepting p-values less than or equal to 0.10 as evidence for rejection of either null hypothesis of non-dispersion, $H_0 : \theta = 0$ for EXCALIBR II or $H_0 : \Delta\mathbf{v} = 0$ for EXCALIBR, inspection of Table 1 shows that EXCALIBR may provide evidence for wrongly rejecting H_0. The p-values provided by EXCALIBR II are statistically valid and thus provide a better measure of dispersion. The results of EXCALIBR II more clearly indicate that wavelength differences of 100 nm or less are insufficient to produce verifiable changes in optic vector positions for the Tiburon albite (Bloss, 1978). Furthermore, EXCALIBR's erroneous rejection of H_0 for the obtuse bisectrix between wavelengths 500 and 600 is absent from the dispersion analysis provided by EXCALIBR II. Thus, EXCALIBR II's dispersion analysis suggesting horizontal dispersion for the Tiburon albite supports the observations reported by Winchell and Winchell (1951).

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