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On the Least-Squares Plane Through a Set of Points*

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A recent discussion by Schomaker *et al.* of the eigenvalue equation determining the best least-squares plane through a set of points is extended. A non-diagonal weight matrix is introduced, the errors associated with the coefficients of the plane are discussed, a criterion for the rejection of a given set as co-planar is given, and a more general form of the equations, valid for the case where certain restrictions are placed on the plane, is presented.

Introduction

In a recent paper, Schomaker, Waser, Marsh & Bergman (1959, hereinafter referred to as SWMB) have presented a derivation of the eigenvalue equation which leads to the best least-squares plane through a set of points. A footnote points out that the weight for an individual point should be chosen inversely proportional to the variance of the perpendicular distance of the point to the plane. It is becoming common practice in the least-squares refinement of atomic positions in crystal structures to invert the complete matrix of coefficients of the normal equations to obtain a variance–covariance matrix (matrix of second moments) which gives not only the errors in the coordinates but their correlations as well. These correlations may well be important in determining the best plane and, in particular, assessing its significance, and it would thus seem desirable to introduce a non-diagonal weight matrix into the scheme of SWMB. It is the main purpose of this paper to present the equations for such an extended treatment and to discuss as well the statistical significance of the results thus obtained.

Notation and mathematical formulation

It is desirable for compactness to use matrix notation throughout.† The following symbols will be used throughout.

$\mathbf{B}_{m,n}$ $\equiv \{b_{ij}\}$, a matrix of m rows and n columns. The subscripts may be omitted after a particular matrix is defined.
B_{ij} or b_{ij}, the element in the ith row and jth column of $\mathbf{B}$.
$\mathbf{B}'_{n,m}$, the transpose of the matrix $\mathbf{B}_{m,n}$.
$\hat{\mathbf{B}}_{n,n}$, the adjoint of a square matrix $\mathbf{B}_{n,n}$.
$\mathbf{B}^{-1}_{n,n}$, the inverse of a square matrix $\mathbf{B}_{n,n}$.
$|\mathbf{B}_{n,n}|$, the determinant of $\mathbf{B}$.
$\mathbf{I}_{n,n}$, a unit matrix.
$\mathbf{O}_{m,n}$, a matrix composed entirely of zeroes.
$\mathbf{a}_j, j=1, 2, \ldots, n$, a linearly independent set of vectors forming the basis for an n-dimensional space.
$\mathbf{G}^{-1}_{n,n}$ $\equiv \{\mathbf{a}_i\cdot\mathbf{a}_j\}$, the metric for this space.
$\mathbf{x}^i_{n,1}$ $\equiv \{x^i_j\}$, a point in this space.
x^i_j, the coordinate of the point $\mathbf{x}^i$ referred to $\mathbf{a}_j$.
$\mathbf{X}_{n,p}$ $\equiv (\mathbf{x}^1\ \mathbf{x}^2\ldots\mathbf{x}^p)$, a set of p points.
$\mathbf{m}_{1,n}$, a vector of coefficients describing the plane

$$\mathbf{m}\mathbf{x}-d=0\,. \quad (1)$$

D^i, the distance of the point $\mathbf{x}^i$ to the plane described by $\mathbf{m}$ and d:

$$D^i=(\mathbf{m}\mathbf{x}^i-d)/(\mathbf{m}\mathbf{G}\mathbf{m}')^{\frac{1}{2}}. \quad (2)$$

$\mathbf{D}_{1,p}$ $\equiv (D^1D^2\ldots D^p)$, the set of p such distances for the points $\mathbf{X}$.

At this point it becomes convenient to introduce the augmented matrices

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† See Hamilton (1954).

$$\mathbf{y}^i_{n+1,1} \equiv \begin{pmatrix} \mathbf{x}^i \\ -1 \end{pmatrix}.$$

$$\mathbf{Y}_{n+1,p} \equiv (\mathbf{y}^1\,\mathbf{y}^2 \ldots \mathbf{y}^p).$$

$$\mathbf{n}_{1,n+1} \equiv (\mathbf{m}\,d).$$

$$\mathbf{H}_{n+1,n+1} \equiv \begin{pmatrix} \mathbf{G}_{n,n} & \mathbf{O}_{n,1} \\ \mathbf{O}_{1,n} & 0 \end{pmatrix}.$$

Equation (1) becomes

$$\mathbf{ny}=0\,, \tag{1a}$$

and the point to plane distance may be written

$$D^i=\mathbf{ny}^i/(\mathbf{nHn}')^{\frac{1}{2}}. \tag{2a}$$

We further define for any set of quantities $q_1, q_2, \ldots, q_r$, a variance–covariance or moment matrix ${}^q\mathbf{M}_{r,r} \equiv \{\sigma_i\sigma_j\varrho_{ij}\}$, where σ_i and σ_j are the standard deviations of the quantities q_i and q_j, and ϱ_{ij} is their correlation coefficient.

Let us now introduce a weight matrix $\mathbf{W}_{p,p}$, whose meaning will be discussed below. Keeping in mind the normalization condition

$$\mathbf{nHn}' \equiv \mathbf{mGm}'=1\,, \tag{3}$$

the function to be minimized may be written

$$F \equiv \mathbf{DWD}'-\lambda[\mathbf{nHn}'-1] \tag{4}$$

and, by methods identical to those of SWMB, we obtain the desired eigenvalue equation:

$$(\mathbf{YWY}'-\lambda\mathbf{H})\mathbf{n}' \equiv (\mathbf{C}-\lambda\mathbf{H})\mathbf{n}'=0.^* \tag{5}$$

The required $\mathbf{n}'$ is the eigenvector corresponding to the minimum eigenvalue λ of (5). This will correspond to the largest eigenvalue of $\hat{\mathbf{C}}\mathbf{H}$; this eigenvalue may be obtained by standard numerical procedures. Less computation is required, however, if we first reduce the secular equation to one of the nth degree by solving the $(n+1)$st equation of (5) to obtain (for $n=3$, for example)

$$\begin{aligned} n_4 \equiv d &= -(1/c_{44})(c_{41}m_1+c_{42}m_2+c_{43}m_3) \\ &\equiv -\boldsymbol{\Gamma}\mathbf{m}'/\gamma \end{aligned} \tag{6}$$

and substitute this value of d in (5). If we partition the matrix $\mathbf{C}$ in the following way:

$$\mathbf{C} \equiv \begin{pmatrix} (\mathbf{XWX}')_{n,n} & \boldsymbol{\Gamma}'_{n,1} \\ \boldsymbol{\Gamma}_{1,n} & \gamma_{1,1} \end{pmatrix} \tag{7}$$

the substitution (6) reduces (5) to

$$[(\mathbf{XWX}'-\boldsymbol{\Gamma}'\boldsymbol{\Gamma}/\gamma)-\lambda\mathbf{G}]\mathbf{m}' \equiv (\mathbf{A}-\lambda\mathbf{G})\mathbf{m}' = 0\,. \tag{8}$$

This is identical to equation (11) of SWMB if the following changes are made in equations (9) and (10) of SWMB to take account of the inclusion of non-diagonal weights.*

$$d = \frac{[w_{kl}x^i_k m_i]}{[w_{kl}]} \equiv m_i\bar{x}^i \qquad \text{SWMB (9)}$$

with

$$\bar{x}^i = \frac{[w_{kl}x^i_k]}{[w_{kl}]}$$

and

$$[w_{kl}X^i_kX^j_l]m_j \equiv A^{ij}m_j = \lambda g^{ij}m_j,\ i=1,\ldots,n \qquad \text{SWMB (10)}$$

with

$$X^i_k \equiv x^i_k-\bar{x}^i.$$

The brackets [ ] now indicate a double summation over all points k and l, and the summation convention is retained for summation over i and j. At this point, the simplification obtained by using matrix notation should be obvious.

Nature of the weight matrix

Now from the general theory of least squares, we know that the weight matrix $\mathbf{W}$ is properly defined by

$$\mathbf{W}_{p,p} \equiv {}^D\mathbf{M}^{-1}_{p,p}\,, \tag{11}$$

where ${}^D\mathbf{M}$ is the moment matrix for the perpendicular distances of the points from the plane. It remains to obtain an expression for ${}^D\mathbf{M}$ in terms of ${}^X\mathbf{M}_{3p,3p}$, the moment matrix for the positional parameters.† From the definition of $\mathbf{D}$, we may write

$$\mathbf{D}'_{p,1}=\begin{pmatrix} \mathbf{m}_{1,3} & \mathbf{O}_{1,3} & \ldots & \mathbf{O}_{1,3} \\ \mathbf{O}_{1,3} & \mathbf{m}_{1,3} & \ldots & \mathbf{O}_{1,3} \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \mathbf{O}_{1,3} & \mathbf{O}_{1,3} & \ldots & \mathbf{m}_{1,3} \end{pmatrix} \begin{pmatrix} \mathbf{x}^1 \\ \mathbf{x}^2 \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{x}^p \end{pmatrix} - d \begin{pmatrix} 1 \\ 1 \\ \cdot \\ \cdot \\ \cdot \\ 1 \end{pmatrix}$$

$$\equiv \mathfrak{M}_{p,3p}\mathfrak{X}_{3p,1}-\mathfrak{D}_{p,1}\,. \tag{12}$$

Hence, by the usual formula for the propagation of error, we obtain

$$\begin{aligned} {}^D\mathbf{M} &= \mathfrak{M}\,{}^X\mathbf{M}\,\mathfrak{M}' \\ &\equiv \{\mathbf{m}({}^X\mathbf{M})^{ij}\mathbf{m}'\}\,, \end{aligned} \tag{13}$$

where $({}^X\mathbf{M})^{ij}$ is the 3×3 block of ${}^X\mathbf{M}$ corresponding to interactions between the points $\mathbf{x}^i$ and $\mathbf{x}^j$. In order to make this point completely clear, we present here the complete expression for the calculation of a single element of ${}^D\mathbf{M}$, viz., the term in the moment matrix for the interaction between points 1 and 2:

* The identity symbol $\equiv$ when used in this way may be interpreted as a definition of $\mathbf{C}$.

* The notation in the remainder of this paragraph is that of SWMB and should not be confused with that of the present paper.

† In this section, we will for clarity confine our discussion to the case of $n=3$. The generalization is obvious.

$$^{D}\mathbf{M}^{12} = (m_1 m_2 m_3) \begin{pmatrix} \sigma(x_1)\sigma(x_2)\varrho(x_1, x_2) & \sigma(x_1)\sigma(y_2)\varrho(x_1, y_2) & \sigma(x_1)\sigma(z_2)\varrho(x_1, z_2) \\ \sigma(y_1)\sigma(x_2)\varrho(y_1, x_2) & \sigma(y_1)\sigma(y_2)\varrho(y_1, y_2) & \sigma(y_1)\sigma(z_2)\varrho(y_1, z_2) \\ \sigma(z_1)\sigma(x_2)\varrho(z_1, x_2) & \sigma(z_1)\sigma(y_2)\varrho(z_1, y_2) & \sigma(z_1)\sigma(z_2)\varrho(z_1, z_2) \end{pmatrix} \begin{pmatrix} m_1 \\ m_2 \\ m_3 \end{pmatrix}.$$

An attempt to introduce the weight matrix in this form into the initial variation problem leads to non-linear equations in $\mathbf{m}$ rather than to the simple eigenvalue expression. The best procedure, as SWMB suggest, would thus seem to be an iterative one, in which one assumes a vector $\mathbf{m}$, calculates the weight matrix from equations (11), (12) and (13), derives a new $\mathbf{m}$, etc. In most cases of interest in two or three dimensions, $\mathbf{m}$ will be approximately known by inspection, so that the process will probably converge in no more than two iterations.

Statistical significance of the derived quantities

Having derived the vector $\mathbf{n}$, we would like to be able to estimate the errors of its components. For this purpose, we require the matrix $^{n}\mathbf{M}$. Since

$$\begin{aligned} \mathbf{Y'n'} &= \mathbf{D'} \\ \mathbf{YWY'n'} &\equiv \mathbf{Cn'} = \mathbf{YWD'} \\ \mathbf{n'} &= \mathbf{C}^{-1}\mathbf{YWD'} \end{aligned} \tag{14}$$

and hence

$$\begin{aligned} ^{n}\mathbf{M} &= \mathbf{C}^{-1}\mathbf{YW}^{D}\mathbf{MWY'C}^{-1} \\ &= \mathbf{C}^{-1}. \end{aligned} \tag{15}$$

Thus, as we expect, the moment matrix for the derived quantities is the inverse of the matrix of the normal equations. Now suppose that we have determined the best vector $\mathbf{n}_0$. We may wish to determine whether another vector $\mathbf{n}$ is also an acceptable solution. If the errors are assumed to be normally distributed, the quantity

$$T^2 = (\mathbf{n}_0 - \mathbf{n})\mathbf{C}(\mathbf{n}_0 - \mathbf{n})' \tag{16}$$

has a distribution of the type originally derived by Hotelling (1931), which in this case may be shown to have the form (Kullback, 1959)

$$T^2 = nF(n, N), \tag{17}$$

where F is the better-known distribution of the ratios of two χ^2 variates. In (17), n is the number of derived parameters (strictly, the rank of $\mathbf{C}$), and N is the number of degrees of freedom which entered into the estimation of $\mathbf{W}$.* (N may be the number of reflections by which a crystal structure is over-determined, for example.) Tables of F are available in most recent statistics texts (see, for example, Adams, 1955). If the value of T^2 calculated by (16) is less than the tabular value for a specified significance level (often 95%), we may conclude that the difference between $\mathbf{n}$ and $\mathbf{n}_0$ is not significant at this level. Since N will be generally large, and since

$$\lim_{N\to\infty} T^2(n, N) = \chi^2(n), \tag{18}$$

the χ^2 test may also be used. Similarly, the quantity $\lambda \equiv \mathbf{D'WD}$ will have the distribution of T^2 with $p-n$ and N degrees of freedom. Here again we may, with little error, use the χ^2 test. If λ is less than the tabulated value of χ^2 for a particular significance level, we may conclude that the deviations from coplanarity are not statistically significant.

All of the conclusions of this section depend upon the proper weights having been used in the derivation of the least-squares plane, and it is primarily for this reason that a correct derivation of the weights is important.

The least-squares plane with conditions

An interesting extension of the problem we have been discussing is that of finding the best plane to fit p points, further requiring that the plane pass exactly through another $l<n$ points. Let the coordinates of these l points be given by $\mathbf{Z}_{n+1,\,l}$ (corresponding to the $\mathbf{Y}_{n+1,\,p}$ for the non-fixed points). The condition may then be expressed

$$\mathbf{nZ} = \mathbf{O}_{1,\,l}\,. \tag{19}$$

The solution of the variation problem (which will not be reproduced here) leads to the result corresponding to (5):

$$\{\mathbf{C} - \lambda[\mathbf{I} - \mathbf{Z}(\mathbf{Z}'\hat{\mathbf{C}}\mathbf{Z})^{-1}\mathbf{Z}'\hat{\mathbf{C}}]\mathbf{H}\}\mathbf{n}' = 0\,. \tag{20}$$

Again the most convenient method of solution is to multiply (20) by $\hat{\mathbf{C}}$ and find the eigenvector corresponding to the largest eigenvalue of the resulting matrix. A substitution similar to that in equation (6) may still be used, but the expression is not quite so straightforward. Perhaps the most common example in three dimensions would be the problem of finding the best plane to fit a given set with the restriction that the plane pass through the origin. Substituting

$$\mathbf{Z}' = (0\ 0\ 0\ -1)$$

in (20), one finds after some manipulation that (20) reduces to

$$(\mathbf{XWX}' - \lambda\mathbf{G})\mathbf{m}' = 0\,, \tag{21}$$

a result that is of course obvious from the fact that $d=0$. If there is only one fixed point, the computational effort will be minimized if one first makes a

* In the usual least-squares adjustment, where the scaling of the weight matrix is dependent on the goodness of fit, the appropriate statistic is of course $T^2 = nF(n, p-n)$, where p is the number of observational equations. This is not the case here, as the normalization of the weight matrix is assumed to arise not from the goodness of fit to the plane but from another source, presumably a least-squares refinement of the atomic positions.

change of origin to this point and then uses (21). The general expression (20) is most useful if there is more than one fixed point, particularly in spaces of higher dimension.

Numerical example

Most of the points in the preceding discussion will now be illustrated by an actual example. For clarity of illustration, let us confine ourselves to a problem with $n=2$, i.e., we are to fit a line to points in the plane.* Let the following four points be given: (0·10, 0·48), (0·73, 0·52), (1·00, 0·70), and (1·30, 0·70). Let us assume further that the axes ($\mathbf{a}_1$ and $\mathbf{a}_2$) are orthogonal with unit length such that

$$\mathbf{H} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Further assume that we have been given a moment matrix for the parameters as follows:

$$^{x}\mathbf{M} = \begin{bmatrix} 0.0100 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.0004 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.0009 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.0064 & 0 & 0.0056 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.0025 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.0056 & 0 & 0.0100 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.0100 & 0.0060 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.0060 & 0.0100 \end{bmatrix}$$

Thus, there is a correlation between the two coordinates of point four, and there is a correlation between the x_2 coordinates of points two and three. The shapes of the error ellipses are shown in Fig. 1. The correlation between points 2 and 3 cannot of course be shown. The analysis follows:

$$\mathbf{Y} = \begin{pmatrix} 0.10 & 0.73 & 1.00 & 1.30 \\ 0.48 & 0.52 & 0.70 & 0.70 \\ -1.00 & -1.00 & -1.00 & -1.00 \end{pmatrix}.$$

Assume as a first approximation that

$$\mathbf{m} = (0.1961 \quad -0.9806)\,.$$

Then

$$^{D}\mathbf{M} = \begin{pmatrix} 769 & 0 & 0 & 0 \\ 0 & 6189 & 5385 & 0 \\ 0 & 5385 & 9712 & 0 \\ 0 & 0 & 0 & 9708 \end{pmatrix} \times 10^6$$

$$\mathbf{W} \equiv {}^{D}\mathbf{M}^{-1} = \begin{pmatrix} 1300 & 0 & 0 & 0 \\ 0 & 312 & -173 & 0 \\ 0 & -173 & 199 & 0 \\ 0 & 0 & 0 & 103 \end{pmatrix}$$

$$\mathbf{YWY}' \equiv \mathbf{C} = \begin{pmatrix} 299.7548 & 235.5022 & -391.3700 \\ 235.5022 & 405.9208 & -786.5800 \\ -391.3700 & -786.5800 & 1568.0000 \end{pmatrix}$$

$$\hat{\mathbf{C}} = \begin{pmatrix} 17775.72 & -61423.64 & -26376.10 \\ -61423.64 & 316845.05 & 143612.63 \\ -26376.10 & 143612.63 & 66215.42 \end{pmatrix}$$

$$|\mathbf{C}| = 11858 \times 10^2$$

$$\hat{\mathbf{C}}\mathbf{H} = \begin{pmatrix} 17775.72 & -61423.64 & 0 \\ -61423.64 & 316845.05 & 0 \\ -26376.10 & 143612.63 & 0 \end{pmatrix}.$$

Choose as a first approximation to the unnormalized $\mathbf{n}$,

$$^{1}\mathbf{n} = (1 \quad -5 \quad \ldots)$$

$$\begin{aligned} \hat{\mathbf{C}}\mathbf{H}\ {}^{1}\mathbf{n}' &= 324894\ (1 \quad -5.065 \quad -2.291)' \equiv 324894\ {}^{2}\mathbf{n}' \\ \hat{\mathbf{C}}\mathbf{H}\ {}^{2}\mathbf{n}' &= 328886\ (1 \quad -5.066 \quad -2.292)' \equiv 328886\ {}^{3}\mathbf{n}' \\ \hat{\mathbf{C}}\mathbf{H}\ {}^{3}\mathbf{n}' &= 328948\ (1 \quad -5.066 \quad -2.292)' \\ \mathbf{n} &= (0.1937 \quad -0.9811 \quad -0.4439) \end{aligned}$$

and the equation of the line is

$$0.1937x - 0.9811y + 0.4439 = 0\,.$$

The values of the coefficients are nearly the same as those used in calculating the weights, so a recycling is not necessary.

$$\lambda = 1185800/328948 = 3.60\,.$$

The value of χ^2 for $p-n=2$ is 5·99 at the 95% level of significance, and therefore any departures from linearity are not statistically significant. In the alternative method of solution indicated in equation (8), we proceed as follows:

$$\begin{aligned} \mathbf{\Gamma} &= (-391.3700 \quad -786.5800) \\ \gamma &= 1568.0000 \\ \mathbf{\Gamma}'\mathbf{\Gamma}/\gamma &= \begin{pmatrix} 97.6853 & 196.3290 \\ 196.3290 & 394.5842 \end{pmatrix} \\ \mathbf{A} &= \begin{pmatrix} 202.0695 & 39.1732 \\ 39.1732 & 11.3366 \end{pmatrix} \\ \hat{\mathbf{A}} &= \begin{pmatrix} 11.3366 & -39.1732 \\ -39.1732 & 202.0695 \end{pmatrix} \\ |\mathbf{A}| &= 756.24 \\ \hat{\mathbf{A}}\mathbf{m}' &= 209.8m' \text{ for } m = (0.1937 \quad -0.9811) \\ \lambda &= 756.24/209.8 = 3.60 \end{aligned}$$

* The three-dimensional case will of course be of most interest to crystallographers. However, in order to present a simple figure, the two-dimensional case has been chosen here. The techniques are of course identical.

which, of course, agrees with the previous results.

As an example of the use of the T^2 test, let us determine the limits of acceptability for lines parallel to the best least-squares line, further assuming that $N=2$, i.e., that our knowledge of the weights is rather poor:

$$(\mathbf{n}-\mathbf{n}_0) = (0 \quad 0 \quad \Delta d)$$
$$T^2 = 1568{\cdot}0\Delta d^2$$
$$T^2 = 2F(2, 2)$$
$$F(2, 2) \text{ at the 95\% confidence level} = 19{\cdot}0\,.$$

Therefore, we must reject any line for which T^2 exceeds $2\times19=38$:

$$1568\Delta d^2 \leq 38$$
$$\Delta d \leq 0{\cdot}16\,.$$

This region of acceptability is indicated in Fig. 1.

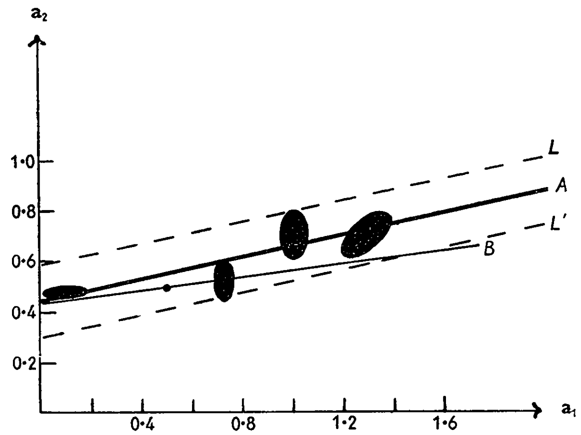

Fig. 1. Illustration of numerical example. The ellipses of standard deviation are indicated. Line A is the best least-squares line without conditions. Line B is the best line which passes through the point $(\frac{1}{2}, \frac{1}{2})$. The two line L and L' are the 95% limits of acceptability for lines parallel to A.

As a final example, let us determine the best line through the same four points, assuming further that the line must pass exactly through the point $(\frac{1}{2}, \frac{1}{2})$:

$$\mathbf{Z}' = (\tfrac{1}{2} \quad \tfrac{1}{2} \quad -1)$$
$$\mathbf{Z}'\mathbf{C}\mathbf{Z} = 1922{\cdot}27$$
$$\mathbf{Z}\mathbf{Z}' = \begin{pmatrix} \frac{1}{4} & \frac{1}{4} & -\frac{1}{2} \\ \frac{1}{4} & \frac{1}{4} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & +1 \end{pmatrix}$$
$$\frac{\mathbf{Z}\mathbf{Z}'\hat{\mathbf{C}}}{\mathbf{Z}'\hat{\mathbf{C}}\mathbf{Z}} = \begin{pmatrix} 1{\cdot}18405 & -4{\cdot}13623 & -1{\cdot}97609 \\ 1{\cdot}18405 & -4{\cdot}13623 & -1{\cdot}97609 \\ -2{\cdot}63810 & 8{\cdot}27246 & 3{\cdot}95218 \end{pmatrix}$$
$$\left[\mathbf{I}-\frac{\mathbf{Z}\mathbf{Z}'\mathbf{C}}{\mathbf{Z}'\mathbf{C}\mathbf{Z}}\right]\mathbf{H} = \begin{pmatrix} -0{\cdot}18405 & 4{\cdot}13623 & 0 \\ -1{\cdot}18405 & 5{\cdot}13623 & 0 \\ 2{\cdot}36810 & -8{\cdot}27246 & 0 \end{pmatrix}$$
$$\hat{\mathbf{C}}\left[\mathbf{I}-\frac{\mathbf{Z}\mathbf{Z}'\hat{\mathbf{C}}}{\mathbf{Z}'\hat{\mathbf{C}}\mathbf{Z}}\right]\mathbf{H} = \begin{pmatrix} 6996 & -23766 & 0 \\ -23766 & 185298 & 0 \\ -8385 & 80766 & 0 \end{pmatrix}$$

and, by a procedure identical to that in the preceding problem, we find

$$\mathbf{n} = (0{\cdot}1299 \quad -0{\cdot}9915 \quad -0{\cdot}4308)$$
$$\lambda = 6{\cdot}3\,.$$

Because of the single restraint, λ is now distributed approximately as χ^2 with three degrees of freedom. Now

$$\chi^2(3) = 7{\cdot}81 \text{ at the 95\% level;}$$

therefore the hypothesis that the points lie on a line passing through the point $(\frac{1}{2}, \frac{1}{2})$ cannot be rejected.

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