atomic scale (111) facets which make up the structure of the (012) plane.

The electron microscope pictures, in addition to confirming the orientations determined by electron diffraction, gave specific data on the shapes of the oxide growth and the particular faces present. Only the three most densely packed faces occurred on the oxide.

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To Fit a Plane or a Line to a Set of Points by Least Squares*

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The fitting of a plane or a line to a set of points by least squares is discussed, and a convenient numerical method is given.

In the description of a crystal structure, it is sometimes desired to fit a least-squares plane to the positions found for some approximately coplanar set of atoms. Because it seems that an incorrect method is often used for doing this, we would like to discuss the problem and recommend an alternative method that is both correct in principle and convenient in computation.

It becomes evident that the problem of the plane is essentially equivalent to the problem of finding the principal plane of least inertia for a set of point masses and that the problem of the best *line* is similarly equivalent to the very closely related problem of the least axis of inertia. The discussion therefore naturally covers line as well as plane and essentially recapitulates parts of a classical mechanical theory in deriving what is special to the present application. We first formulate the problem of the plane and present the recommended alternative method of solution, including a detailed numerical example, then discuss the prevalent incorrect method as well as various special cases, and finally consider the problem of the line and give a convenient method for handling it.

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We find it convenient to use both ordinary vector notation, as in equations (1), (2), and (3), and matrix notation, as in equation (11), sometimes side by side. We also use two summation conventions: the Gaussian bracket [ ], to express summation over a set of points (cf., e.g., Whittaker & Robinson, 1940), and the convention of dropping the operator Σ whenever it applies to repeated alphabetic indices. Definitions we often express as identities.

The least-squares plane

What is desired is to find the plane that minimizes $S \equiv \Sigma_k w_k D_k^2 \equiv [wD^2]$, the weighted sum of squares of distances D_k of points k from the plane sought. These points are defined by the vectors

$$\mathbf{r} \equiv x^1\mathbf{a}_1 + x^2\mathbf{a}_2 + x^3\mathbf{a}_3 \equiv x^i\mathbf{a}_i \,. \qquad (1)$$

The plane is defined by its unit normal

$$\mathbf{m} \equiv m_1\mathbf{b}^1 + m_2\mathbf{b}^2 + m_3\mathbf{b}^3 \equiv m_i\mathbf{b}^i \qquad (2)$$

and by the origin-to-plane distance d, whereupon the distance from the plane to a point is

$$\mathbf{m}.\mathbf{r} - d \equiv m_i x^i - d \qquad (3)$$

and the weighted* sum of squares of residuals is

$$S \equiv [wD^2] \equiv [w(m_i x^i - d)^2] \,. \tag{4}$$

The condition that $\mathbf{m}$ be a unit vector is expressed by

$$\mathbf{m}.\mathbf{m} \equiv \mathbf{b}^i.\mathbf{b}^j m_i m_j \equiv g^{ij} m_i m_j = 1 \,. \tag{5}$$

To make S stationary subject to this condition, one introduces a Lagrange multiplier λ and writes a composite expression

$$F \equiv [w(m_i x^i - d)^2] - \lambda g^{ij} m_i m_j \,, \tag{6}$$

which leads directly to the normal equations,

$$\frac{1}{2}\frac{\partial F}{\partial m_i} = [w x^i (m_j x^j - d)] - \lambda g^{ij} m_j = 0, \quad i = 1, 2, 3 \tag{7}$$

$$-\frac{1}{2}\frac{\partial F}{\partial d} = [w(m_j x^j - d)] = 0 \,. \tag{8}$$

The last equation is solved by

$$d = [w m_j x^j]/[w] = m_j \overline{x^j} \,, \quad \text{with} \quad \overline{x^j} \equiv [w x^j]/[w], \tag{9}$$

which shows that transformation to the coordinates $X^i \equiv x_i - \overline{x_i}$ eliminates d and reduces the three equations (7) to the form

$$[w X^i X^j] m_j \equiv A^{ij} m_j = \lambda g^{ij} m_j, \quad i = 1, 2, 3 \,. \tag{10}$$

In matrix notation this corresponds to

$$\mathrm{Am} = \lambda \mathrm{gm} \,, \tag{11}$$

while (4) and (5) become

$$S \equiv \tilde{\mathrm{m}}\mathrm{Am}; \quad \tilde{\mathrm{m}}\mathrm{gm} = 1 \,, \tag{12}$$

where m and $\tilde{\mathrm{m}}$ are representations of the vector $\mathbf{m}$ by column and row matrices, respectively. Equation (11) is an eigenvalue equation, satisfied only if λ is an eigenvalue $\lambda^{(i)}$; for a given $\lambda^{(i)}$ the matrix solution m of this equation is an eigenvector $\mathrm{m}^{(i)}$. The familiar determinantal equation $|\mathrm{A} - \lambda \mathrm{g}| = 0$, a cubic equation in λ, leads to the three roots $\lambda^{(1)} \ll \lambda^{(2)} \leq \lambda^{(3)}$, corresponding to the *best* plane, an intermediate plane, and a 'worst' plane, all at right angles to one another. All these planes go through the centroid, and, as will be seen later, the 'worst' plane is perpendicular to the best line that can be drawn through the points. Except for the substitution of *weights* for masses the situation is indeed that of the principal planes of inertia for the same set of atoms. The orientational part of the transformation has recently been discussed for the general case of triclinic axes using the temperature factor as an example (Waser, 1955).

The meaning of the eigenvalue $\lambda^{(1)}$ becomes clear if the equation $\mathrm{Am}^{(1)} = \lambda^{(1)}\mathrm{gm}^{(1)}$ is multiplied from the left by $\tilde{\mathrm{m}}^{(1)}$:

$$\tilde{\mathrm{m}}^{(1)}\mathrm{Am}^{(1)} = \lambda^{(1)}\tilde{\mathrm{m}}^{(1)}\mathrm{gm}^{(1)} = \lambda^{(1)} \,. \tag{13}$$

Since the left side also equals S, $\lambda^{(1)}$ is the minimum value of the sum of residuals; in particular, exact coplanarity corresponds to $\lambda^{(1)} = 0$. The eigenvalues $\lambda^{(2)}$ and $\lambda^{(3)}$ have analogous meanings. It will be noted that approximate collinearity corresponds to $\lambda^{(1)} \approx \lambda^{(2)} \ll \lambda^{(3)}$, and exact collinearity to $\lambda^{(1)} = \lambda^{(2)} = 0$.

Iterative numerical solution

While the standard eigenvalue problem involves the solution of a cubic determinantal equation in addition to a set of simultaneous linear equations for the components of the eigenvectors, the present problem of the plane, by virtue of the smallness of the crucial eigenvalue $\lambda^{(1)}$ (i.e., by virtue of the goodness of fit of the points to the plane, relative to their extension in the plane), can be simply and effectively handled by iteration (cf., e.g., Frazer, Duncan & Collar, 1938). The basic relation for this is

$$\mathrm{Bm} \equiv \hat{\mathrm{A}}\mathrm{gm} = (|A|/\lambda)\mathrm{m} \,. \tag{14}$$

It is obtained by multiplying (11) from the left with $\hat{\mathrm{A}}$ (the adjoint matrix of A), using the property $\hat{\mathrm{A}}\mathrm{A} = |\mathrm{A}|\mathrm{I}$, and writing B for $\hat{\mathrm{A}}\mathrm{g}$. It follows from this relation that almost any initially chosen vector $\mathrm{m}_{(0)}$ is transformed into a multiple of the eigenvector $\mathrm{m}^{(1)}$ by a sufficient number of repeated multiplications by the matrix B: we first express $\mathrm{m}_{(0)}$ in terms of the eigenvectors $\mathrm{m}^{(i)}$,

$$\mathrm{m}_{(0)} = c_1\mathrm{m}^{(1)} + c_2\mathrm{m}^{(2)} + c_3\mathrm{m}^{(3)} \,, \tag{15}$$

and then multiply repeatedly with B to obtain

$$\begin{aligned} \mathrm{m}_{(1)} \equiv \mathrm{Bm}_{(0)} &= c_1(|\mathrm{A}|/\lambda^{(1)})\mathrm{m}^{(1)} \\ &\quad + c_2(|\mathrm{A}|/\lambda^{(2)})\mathrm{m}^{(2)} + c_3(|\mathrm{A}|/\lambda^{(3)})\mathrm{m}^{(3)} \\ &\cdots\cdots \\ \mathrm{m}_{(n)} \equiv \mathrm{Bm}_{(n-1)} &= c_1(|\mathrm{A}|/\lambda^{(1)})^n\mathrm{m}^{(1)} \\ &\quad + c_2(|\mathrm{A}|/\lambda^{(2)})^n\mathrm{m}^{(2)} + c_3(|\mathrm{A}|/\lambda^{(3)})^n\mathrm{m}^{(3)} \\ &\approx c_1(|\mathrm{A}|/\lambda^{(1)})^n\mathrm{m}^{(1)} \,. \end{aligned}$$

For a typical 'good' plane $\lambda^{(1)}/\lambda^{(2)}$ and $\lambda^{(1)}/\lambda^{(3)}$ will probably be of the order of 10^{-4} (average distance of points from plane 0·01 Å, average distance of points from centroid 1 Å). Almost any $\mathrm{m}_{(0)}$ will then converge to c_1 $(|\mathrm{A}|/\lambda^{(1)})\mathrm{m}^{(1)}$ with rather high precision in one step, so that a second multiplication by B is necessary

* If the weights for different points have ratios $w_k/w_{k'}$ invariant to the orientation of the desired plane, the weights may be taken as constants, even though the relevant prescription $w \propto 1/\sigma_\perp^2$ ($\sigma_\perp$ for any point is the standard error of the component of $\mathbf{r}$ perpendicular to the plane) might seem to suggest otherwise if $\sigma_\perp^2$ is anisotropic. If the ratios are not invariant, on the other hand, the weights have to be adjusted to conform to the actual orientation of the plane, perhaps in successive stages of approximation. Our general discussion presumes constant ratios; it could be applied, however, to the successive stages of the refinement for the non-constant case.

Of course, it may be desired to use least squares for finding a best plane in a purely formal sense (without regard to the accuracies of the $\mathbf{r}_k$), taking, for example, unit weights.

only to verify and refine the convergence and to evaluate $|A|/\lambda^{(1)}$. The exceptional case would be the unfortunate one of $c_1 \approx 0$, whereupon $m_{(n)} \approx c_1(|A|/\lambda^{(1)})^n m^{(1)}$, though still a true equation, no longer provides an approximation to $m^{(1)}$, being essentially of the form $0 \approx 0.m^{(1)}$.

Therefore, consider as choice for $m_{(0)}$ one of the three vectors

$$\begin{pmatrix}1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\end{pmatrix} \quad \text{and} \quad \begin{pmatrix}0\\0\\1\end{pmatrix}.$$

The vector $Bm_{(0)}$ is then a column vector of B. Due to the rapid convergence just envisioned, this column vector will be almost parallel to $m^{(1)}$, which is to say the column vectors of B are themselves almost parallel. The exceptional case in which $m_{(0)}$ is almost orthogonal to $m^{(1)}$ and corresponds to a very small value of c_1 can then be quickly recognized, since it corresponds to a very small column vector of B: the expansion of this vector by equation (15) will have all three coefficients small because they contain as factors c_1, $1/\lambda^{(2)}$, and $1/\lambda^{(3)}$, respectively. The rule thus emerges that a uniformly good choice of $Bm_{(0)}$ is the largest column vector of B.

If the fit of points to plane is perfect, $S_{\min.}$ and thus $\lambda^{(1)}$ are zero, so that $|A|$ is zero also, being the constant term $\lambda^{(1)}\lambda^{(2)}\lambda^{(3)}$ in the foregoing determinantal equation. This has the consequence that the column vectors of $\hat{A}$ become strictly proportional to one another (cf., e.g., Frazer, Duncan & Collar, 1938), which is to say that $\hat{A}_{ij}$ takes the form $\hat{A}_{ij} = r_i s_j$. (For later purposes we mention that any matrix of rank 1 shows this behavior, and inversely.) This property is transferred to $B(B_i^k \equiv \hat{A}_{ij}g^{jk} \equiv r_i s_j g^{jk} \equiv r_i t^k)$ and has the further consequence that $m^{(1)}$ is strictly proportional to the column vectors $t^k\mathbf{r}$ of B. Indeed, $m_i^{(1)} = (\lambda^{(1)}/|A|)B_i^k m_k^{(1)} = \text{const.}\, r_i t^k m_k = \text{const.}\, r_i$. We note that even in the case just considered the quantity $|A|/\lambda^{(1)}$ in equation (14) remains finite, being equal to $\lambda^{(2)}\lambda^{(3)}$. However, if the points are precisely collinear, $|A|/\lambda^{(1)}$ is equal to zero, and, moreover, $\hat{A}$ is a null matrix.

In practice one evaluates the coordinates of the centroid $\overline{x^i} = [wx^i]/[w]$; forms $A = ([wx^ix^j] - [wx^i]\overline{x^j})$, the adjoint matrix $\hat{A}$ (which has as ij element $(-1)^{i+j}$ times the subdeterminant associated with the ji element in A), $\hat{A}A = |A|I$ (to determine $|A|$ and check the computation of $\hat{A}$), and $B = \hat{A}g$; chooses the largest column vector of B for $m_{(1)} = Bm_{(0)}$; multiplies with B until the ratios $m_{i(n)}/m_{i(n-1)}$, $i = 1, 2, 3$, are equal to one another and have thus attained their limiting value $|A|/\lambda^{(1)}$; normalizes m by $\tilde{m}gm = 1$; and evaluates $d = m_j\overline{x^j}$ and the residuals $m_jx^j - d$. These must stand reasonable scrutiny and have weighted sum of squares equal to $\lambda^{(1)}$.

Numerical example

A practical example (the benzene ring in the phenyl cyclobutenedione structure at its present stage of refinement; C. Wong, R. E. Marsh & V. Schomaker, to be published) will serve to illustrate some of the foregoing considerations as well as show that the recommended procedure is actually quite simple. Table 1 reproduces all that had to be recorded—except for familiar steps leading to the b^i—when the work was done on a desk calculator.

Discussion

While the foregoing approach is based on the equation of a plane in the form $m_ix^i = d$ (cf. equations (1) to (4)), this equation can be written also in its 'normal' form

$$(m_i/d)x^i = n_ix^i = 1\,,$$

where the n_i are independent and where $g^{ij}n_in_j = 1/d^2$. (It is already apparent that difficulties will arise when d approaches zero.)

If one now asks for the 'best' values for the n_i to fit a set of points $\mathbf{r}_k$, one may be led to the criterion

$$[w(n_ix^i - 1)^2] = \text{min.}\,,$$

which corresponds to the minimization of $S/d^2 \equiv [w(D/d)^2]$ rather than of S. If d is large compared with the deviations of the points from the plane, the resulting plane will be close to the one obtained by minimizing S; however, if d is small (or the points badly non-planar, or the lateral distance of the origin from the centroid relatively great), the resulting plane may be significantly in error. The origin effectively repels the plane with a force depending inversely on the origin-to-plane distance, causing the plane to translate and (in general) rotate away from its proper position. Approximate expressions for the magnitudes of these effects will now be derived.

While minimization of S/d^2 leads directly to the normal equations

$$[wx^ix^j]n_j = [wx_i], \quad i = 1, 2, 3 \tag{16}$$

or in matrix notation

$$\alpha\mathrm{n} = \xi\,, \tag{17}$$

the problem will be treated differently, for purposes of comparison. If the conditions for S/d^2 stationary subject to $g^{ij}m_im_j = 1$ are written out in analogy to (7) and (8) with Lagrange multiplier μ, the equations

$$Am - \mu d^2 \mathrm{gm} = (S/d)\overline{\mathrm{x}}$$
$$d = m_i\overline{x^i} + S/[w]d$$

can be readily obtained. These equations can be solved for our case of interest as a perturbation problem by regarding $(S/d)\overline{\mathrm{x}}$ as a small perturbation of the

Table 1. *Numerical example of least-square plane*

Unit weights. Data in italics, results in bold-face

Atom	x^1	x^2	x^3	D (Å)	D^* (Å)
1	*0·1780*	*0·5356*	*0·3731*	**0·0030**	0·0051
2	*0·1389*	*0·6645*	*0·3177*	**0·0034**	0·0048
3	*0·1670*	*0·7929*	*0·3765*	**−0·0049**	−0·0054
4	*0·2370*	*0·7882*	*0·4918*	**0·0000**	−0·0017
5	*0·2786*	*0·6594*	*0·5498*	**0·0062**	0·0049
6	*0·2447*	*0·5311*	*0·4867*	**−0·0079**	−0·0070
[ ]	1·2442	3·9717	2·5956	**−0·0002**	0·0007
$\overline{x^i}$	0·2073⅔	0·6619½	0·4326	—	—

$a_1 = 7{\cdot}000$ Å
$a_2 = 9{\cdot}287$ Å
$a_3 = 12{\cdot}340$ Å
$\beta = 103{\cdot}31°$
$b^1 = 0{\cdot}14680$ Å^{-1}
$b^2 = 0{\cdot}10768$ Å^{-1}
$b^3 = 0{\cdot}08327$ Å^{-1}
$b^3 \sin\beta = 0{\cdot}01917$ Å^{-1}

100A

1·4525653	−0·3075630	2·4001280
−0·3075630	6·6186015	−0·0025310
2·4001280	−0·0025310	4·0056760

10^9ÂA

7·973	0·000	0·002
0·000	7·975	0·000
0·001	0·001	7·973

10^3Â

2·6511967	0·1225923	−1·5884712
0·1225923	0·0057892	−0·0734514
−1·5884712	−0·0734514	0·9519356

10g

0·21550	0	0·02814
0	0·11595	0
0·02814	0	0·06934

10^5B

5·2663	0·1421	−0·3554
0·2435	0·0067	−0·0164
−3·1553	−0·0852	0·2131

10^5m$_{(0)}$	10^{10}m$_{(1)}$	m$^{(1)}$
5·2663	28·890	**6·9518**
0·2435	1·336	**0·3215**
−3·1553	−17·310	**−4·1653**

$10^5 m_{i(1)}/m_{i(0)}$: 5·4858, 5·4867, 5·4858

$\lambda^{(1)} = 7{\cdot}97\times10^{-9}/5{\cdot}49\times10^{-5} = \mathbf{1{\cdot}45\times10^{-4}}$

S (from D, above) $= \mathbf{1{\cdot}45\times10^{-4}}$

10^{11}gm$_{(1)}$: 5·7387, 0·1549, −0·3873

$10^{20}\tilde{m}_{(1)}$gm$_{(1)} = 17{\cdot}270$; $(17{\cdot}270)^{-\frac{1}{2}} = 0{\cdot}24063$

$d = \tilde{m}^{(1)}\bar{x} = \mathbf{-0{\cdot}1475}$ Å

* For plane obtained by the incorrect method; see Discussion.

previous eigenvalue equation $Am-\lambda gm = 0$. We write $m = m^{(1)}+m'$ and $\mu d^2 = \lambda^{(1)}+\lambda'$ and find the following first-order results of interest. The twist of the plane from its correct orientation is described by

$$m' = \tilde{m}^{(2)}\bar{x}\frac{S}{d(\lambda^{(2)}-\lambda^{(1)})}m^{(2)}+\tilde{m}^{(3)}\bar{x}\frac{S}{d(\lambda^{(3)}-\lambda^{(1)})}m^{(3)}$$
$$\approx \tilde{m}^{(2)}\frac{\bar{x}\lambda^{(1)}}{d\lambda^{(2)}}m^{(2)}+\tilde{m}^{(3)}\frac{\bar{x}\lambda^{(1)}}{d\lambda^{(3)}}m^{(3)},$$

while the translation of the plane is described by

$$d' \equiv d-d^{\text{correct}} = \tilde{m}'\bar{x}+S/[w]d$$
$$\approx \frac{(\tilde{m}^{(2)}\bar{x})^2\lambda^{(1)}}{d\lambda^{(2)}}+\frac{(\tilde{m}^{(3)}\bar{x})^2\lambda^{(1)}}{d\lambda^{(3)}}+\frac{\overline{D^2}}{d},$$

where in the last line we have written $\overline{D^2}$, the mean squared residual, for $S/[w]$. In terms of the deviation of a given point from the plane, the difference between the two methods is given by

$$D' \equiv D-D_{\text{correct}}$$
$$= \tilde{m}x-d-(\tilde{m}^{(1)}x-d_{\text{correct}}) = \tilde{m}'X-S/[w]d$$
$$\approx \tilde{m}^{(2)}\frac{\bar{x}\lambda^{(1)}}{d\lambda^{(2)}}\tilde{m}^{(2)}X+\tilde{m}^{(3)}\frac{\bar{x}\lambda^{(1)}}{d\lambda^{(3)}}\tilde{m}^{(3)}X-\frac{\overline{D^2}}{d}.$$

Alternative expressions without explicit reference to $\lambda^{(2)}$, $\lambda^{(3)}$, $m^{(2)}$, and $m^{(3)}$ can also be found; the key expression is

$$m' = Sd^{-1}(1-m^{(1)}\tilde{m}^{(1)}g)A^{-1}\bar{x}.$$

It will be easy to see that in any practical case the method involving (16) or (17) may be satisfactory or not depending on the values of $\bar{x}/d$, $\overline{D^2}/d$, $\lambda^{(1)}/\lambda^{(2)}$, and $\lambda^{(1)}/\lambda^{(3)}$, as well as the criteria to be used for judging the resulting errors m', d', and D'.

When the benzene ring of phenyl cyclobutenedione was treated by the incorrect method, the first difficulty was in solving equations (17): they are badly ill-conditioned, and winning an adequate solution of them was much more troublesome than carrying out the full recommended procedure. Moreover, the plane is indeed twisted and displaced, as is shown by the origin-to-plane distance, 0·1588 Å, and the D values, which are given in the Table. Of course, as seems to have been belatedly discovered several times before, the origin can be moved if trouble threatens—moved away from the plane and toward the normal passing through the centroid—and our approximate relations could serve as a guide in this respect. But there would always be some residual error, and, for all that we understand of it, the ill-conditioning would remain in doubt.

A final point about the plane is that, if Cartesian coordinates (for which g is the unit matrix) have already been introduced, our B will coalesce with $\hat{\mathrm{A}}$. The essence of the work is then expressed by the equation $\mathrm{Am}_{(0)} \approx \text{const.}\, \mathrm{m}^{(1)}$ with the largest column vector of A as the logical choice for $\mathrm{m}_{(0)}$.

The least-squares line

The problem of the best plane is closely related to the problem of the best line through a set of points. It may be obvious, from the close analogy to the problem of the least axis of inertia or otherwise, that this line passes through the centroid and is perpendicular to what we have called the worst plane. Nevertheless, the following formal demonstration may not be out of place.

We first derive an expression for the distance of the point described by the vector $\mathbf{x} = x^i\mathbf{a}_i$ from a line which passes through the point $\mathbf{x}_0 = x_0^i\mathbf{a}_i$ and is parallel to the unit vector $\mathbf{m} = m_i\mathbf{b}^i$. This line can be described by the equation

$$\mathbf{r} = \mathbf{x}_0 + t\mathbf{m}\,, \tag{18}$$

where t is a parameter which can assume all real values. The square of the distance D from point to line is equal to the square of the distance $|\mathbf{x}_0-\mathbf{x}|$ diminished by the square of the projection of this distance on the line (18):

$$D^2 = (\mathbf{x}_0-\mathbf{x})^2-(\mathbf{m}\,.\,(\mathbf{x}_0-\mathbf{x}))^2 = (x_0^i-x^i)(x_0^j-x^j)(g_{ij}-m_im_j)\,,$$

with $g_{ij} = \mathbf{a}_i\,.\,\mathbf{a}_j$.

If now a number of points are to be fitted by a best line, the problem is readily put in the form of finding the parameters x_0^i and m_i which make

$$S' = [w(x_0^i-x^i)(x_0^j-x^j)](g_{ij}-m_im_j)$$

a minimum, subject to the auxiliary condition (5). We use again a Lagrange multiplier λ and find eventually the equations

$$x_0^i = \overline{x^i};\quad [wx^ix^j]m_j \equiv A^{ij}m_j = \lambda g^{ij}m_j;\quad i = 1, 2, 3\,. \tag{19}$$

The line sought thus goes through the centroid, and the conditions on m are precisely those of equations (10) or (11), or also $\mathrm{g}^{-1}\mathrm{Am} = \lambda\mathrm{m}$. The sum of the residuals can be expressed in the form

$$S'^{(i)} = \mathrm{Spur}\,\mathrm{g}^{-1}\mathrm{A}-\tilde{\mathrm{m}}^{(i)}\mathrm{Am}^{(i)} = \sum_k \lambda^{(k)}-\lambda^{(i)}(\geq 0)\,.$$

It is clear that the situation concerning the eigenvalues and eigenvectors is just the opposite of the one for the plane. The largest eigenvalue, $\lambda^{(3)}$, is associated with an absolute minimum of S'; its eigenvector $\mathrm{m}^{(3)}$ is parallel to the best line (and perpendicular to the 'worst' plane) while the other two eigenvectors correspond to an 'intermediate' and a 'worst' line (perpendicular to the 'intermediate' and the best plane, respectively). One can speak of an effective fit of a line to the points only when $\lambda^{(3)} \gg \lambda^{(2)}, \lambda^{(1)}$. When looking for the best line to fit a set of points one will thus conveniently use the matrix $\mathrm{g}^{-1}\mathrm{A}$ rather than the matrix B employed previously, which is essentially its inverse.

For the case of a perfect fit $|\mathrm{A}-\lambda\mathrm{g}| = 0$ has a double root zero, the double degeneracy corresponding to the infinitely many planes passing through the line. Because of this double degeneracy, A and thus $\mathrm{g}^{-1}\mathrm{A}$ have rank 1. The column vectors of $\mathrm{g}^{-1}\mathrm{A}$ are therefore parallel to one another and to $\mathrm{m}^{(3)}$.

The equation of the line sought is

$$\mathbf{r} = \overline{\mathbf{r}}+t\mathbf{m}^{(3)},$$

since it passes through the centroid $\overline{\mathbf{r}}$, or, by virtue of $b^i = g^{ij}a_j$,

$$x^i = \overline{x^i}+tm_j^{(3)}g^{ji};\quad i = 1, 2, 3\,.$$

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