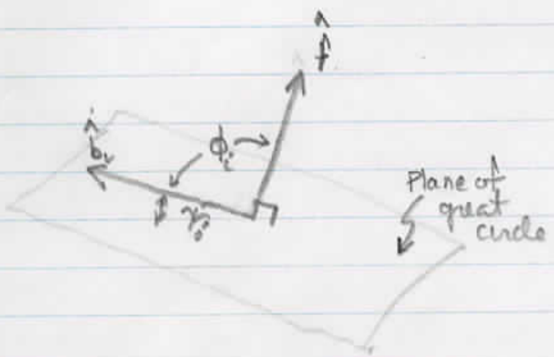
Ramsey's and Watson's methods of fitting great circles:

1\. Both authors start by defining a unit vector, say $\hat{f}$ which points along the fold axis, and a set of unit vectors, say $\hat{b}_i$ which point to poles of bedding. The angle between the bedding pole and the fold axis is called ϕ_i, the angle between the bedding pole and the plane of the great circle is called γ_i.



2\. if $\hat{f}$ has components (p, q, r) (which are to be determined) and

$\hat{b}_i$ has components (l_i, m_i, n_i) (which are known, the data)

vector analysis gives:

$$\sin \gamma_i = \cos \phi_i = \hat{f} \cdot \hat{b}_i = (l_i p + m_i q + n_i r)$$

3\. if the bedding pole was exactly on the plane of the great circle, then $\phi_i = 90°$ and $\gamma_i = 0°$. But we expect scatter of the bedding poles, so we choose to find the components of $\hat{f}$ which minimize:

$$\text{ERROR} = E = \sum_i (\sin \gamma_i)^2 = \sum_i (l_i p + m_i q + n_i r)^2$$

4\. Now here's the part that Ramsey gets wrong. Not any choice of p, q, r that minimizes the error will do. p, q and r are components of a <u>unit</u> vector, and therefore

$$\text{Length of } \hat{f} = p^2 + q^2 + r^2 = 1$$

5. The least squares problem can then be stated ;

find the p, q, r which minimizes $\text{Error} = E = \Sigma \, (p l_i + q m_i + r n_i)^2$

subject to the constraint that $L = p^2 + q^2 + r^2 - 1 = 0$

6. This problem is conviently solved by the method of Lagrange multipliers. This method defines an (as yet unknown) parameter λ. It the asserts that the solution to 5) is given by :

solve simultaneously :
$$\frac{\partial E}{\partial p} - \lambda \frac{\partial L}{\partial p} = 0$$

$$\frac{\partial E}{\partial q} - \lambda \frac{\partial L}{\partial q} = 0$$

$$\frac{\partial E}{\partial r} - \lambda \frac{\partial L}{\partial r} = 0$$

7. The equations in 6) can be written as :

$$\begin{pmatrix} \Sigma l_i^2 & \Sigma l_i m_i & \Sigma l_i n_i \\ \Sigma l_i m_i & \Sigma m_i^2 & \Sigma m_i n_i \\ \Sigma l_i n_i & \Sigma m_i n_i & \Sigma n_i^2 \end{pmatrix} \begin{pmatrix} p \\ q \\ r \end{pmatrix} = \lambda \begin{pmatrix} p \\ q \\ r \end{pmatrix} \quad \text{or } M\hat{f} = \lambda \hat{f}$$

8. The matrix equation is 7) is in the form of a standard eigenvalue - eigenvector equation well known to mathematics. It has three solutions :

$$\lambda_1 , \begin{pmatrix} p_1 \\ q_1 \\ r_1 \end{pmatrix} \qquad \lambda_2 , \begin{pmatrix} p_2 \\ q_2 \\ r_2 \end{pmatrix} \qquad \lambda_3 , \begin{pmatrix} p_3 \\ q_3 \\ r_3 \end{pmatrix}$$

One solution minimizes the error. One solution maximizes the error. One solution is an inflection point in the error. The solution with smallest λ is the one we want, the one which minimizes the error.

9. The residual sum of squares. suppose that we have chosen the (p, q, r) which minimize the error. Then the error is given by :

$$E = \Sigma (p l_i + q m_i + r n_i)^2 = \Sigma (p^2 l_i^2 + q^2 m_i^2 + r^2 n_i^2 + 2pq\, l_i m_i +$$

$$2pr\, l_i n_i + 2qr\, m_i n_i) = p^2 \Sigma l_i^2 + q^2 \Sigma m_i^2 + r^2 \Sigma n_i^2 + 2pq \Sigma l_i m_i$$

$$+ 2pr \Sigma l_i n_i + 2qr \Sigma m_i n_i$$

Thus the error can be written as the matrix form :

$$E = (p \ q \ r) \begin{pmatrix} \Sigma l_i^2 & \Sigma l_i m_i & \Sigma l_i n_i \\ \Sigma l_i m_i & \Sigma m_i^2 & \Sigma m_i n_i \\ \Sigma l_i n_i & \Sigma m_i n_i & \Sigma n_i^2 \end{pmatrix} \begin{pmatrix} p \\ q \\ r \end{pmatrix}$$

$$= \hat{f}^T M \hat{f}$$

but we have chosen the $\hat{f} = (p, q, r)$ which satisfies $M\hat{f} = \lambda \hat{f}$ so that $E = \hat{f}^T M \hat{f} = \hat{f}^T \lambda \hat{f} = \lambda \hat{f}^T \hat{f} = \lambda$, since $\hat{f}^T \hat{f} = p^2 + q^2 + r^2 = 1$. so finally, the residual error is given by :

$$\text{Error} = E = \lambda$$

so that λ has a simple, physical interpretation as the error or residual sum of squares.

ERROR analysis. FOLLOWING ASSUMPTIONS MADE.

1. The errors the measurement of the strike and dip (Ψ) of any single bedding plane are known (or can be conviently estimated). This error is represented by the covariance matrix $\mathrm{cov}(\Psi_i, \Psi_j)$. The errors from bedding plane to bedding plane are completely uncorrelated.

2. The errors are small (so that functions can be represented by taylor series containing only the first power of the error.

statement of problem

1. given the covariance matrices of the data: $\mathrm{cov}(\Psi_i, \Psi_j)$ find the covariance matrix of the bearing and plunge of the best fit plane's normal (Φ), $\mathrm{cov}(\Phi_i, \Phi_j)$

general proceedure

1. we will make much use of the following rule for working with covariances:

given some functions $f_i(x_j)$ where the x_j are known only within some tollerance, say δx_j then if we can write:

$$f_i(x_j) = f_i^\circ(x_j^\circ) + \sum_j \left.\frac{\partial f_i}{\partial x_j}\right|_{x^\circ} \delta x_j$$

$$= f_i^\circ(x_j) + \sum_j a_{ij}\, \delta x_j$$

Then approximately :

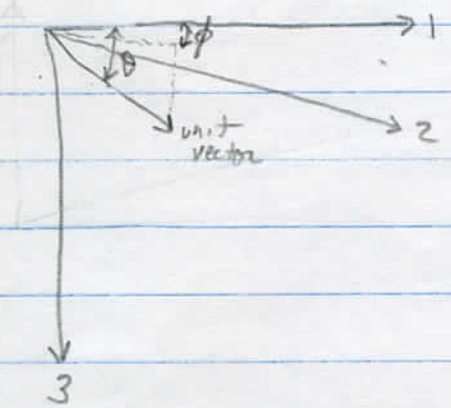
$$\mathrm{cov}(f_i, f_j) \approx \sum_k \sum_l a_{ik}\, \mathrm{cov}(X_k, X_l)\, a_{jk}$$

<u>specific procedure</u>

1. we start with the covariance in the data $\mathrm{cov}(\gamma_i, \gamma_j)$
2. we compute the covariance of the matrix of products of unit vector components (for one bedding plane) $\mathrm{cov}(d_i, d_j)$ by expanding the relations between the (bearing, plunge) data and the matrix elements, This relation is approx.
   $d_i = d_i^\circ + \sum e_{ij}\, \delta \gamma_j$
3. we recognize that since the data for different bedding planes is completely uncorrellated, the covariance of the matrix of sums of products is the sum of the covariances of the individual matrices. $\mathrm{cov}(b_i, b_j) = \sum_{\text{data}} \mathrm{cov}(d_i, d_j)$
4. we map the covariance of matrix elements into covariance of eigenvector (fold axis unit vector) components $\mathrm{cov}(f_i, f_j)$ using a perturbation expansion given by wilkenson. The expansion leads to $f_i \approx f_i^\circ + \sum_k \xi_{ik}\, \delta b_k$
5. we map the covariance in the unit vector into the covariance in the (bearing, plunge) $= \Phi$ of the fold axis by a taylor series expansion of the cartesian to polar transformations. $\Phi_i \approx \Phi_i^\circ + \sum t_{ij}\, \delta f_j$.

Suppose data is a list of vectors $\psi_j^{(i)} = [\phi_i, \theta_i]$, i over data

Then let these have unit vectors (l, m, n) with



$(1,2,3) \equiv$ (NORTH, EAST, DOWN)

$(\phi_i, \theta_i) \equiv$ (bearing N of E, plunge)

$$l = \cos\phi \cos\theta$$
$$m = \sin\phi \cos\theta$$
$$n = \sin\theta$$

Then around a point (θ_0, ϕ_0) we have by taylor's thm:

$$l \approx \cos\phi_0 \cos\theta_0 - \sin\phi_0 \cos\theta_0 \, \delta\phi - \cos\phi_0 \sin\theta_0 \, \delta\theta$$

$$m \approx \sin\phi_0 \cos\theta_0 + \cos\phi_0 \cos\theta_0 \, \delta\phi - \sin\phi_0 \sin\theta_0 \, \delta\theta$$

$$n \approx \sin\theta_0 + 0 + \cos\theta_0 \, \delta\theta$$

then suppose these are formed into products

$$d = [l^2, lm, ln, m^2, mn, n^2]$$

We can write then that:

$$d_i = d_i^0 + \sum_{j=1}^{2} e_{ij} \, \delta\psi_j$$ where e_{ij} is given by

$$e_{ij} = \begin{bmatrix} (-2\cos\phi\sin\phi\cos^2\theta) & (-2\cos^2\phi\cos\theta\sin\theta) \\ ((\cos^2\phi - \sin^2\phi)\cos^2\theta) & (-2\cos\phi\sin\phi\cos\theta\sin\theta) \\ (-\sin\phi\cos\theta\sin\theta) & (\cos\phi(\cos^2\theta - \sin^2\theta)) \\ (2\cos\phi\sin\phi\cos^2\theta) & (-2\sin^2\phi\cos\theta\sin\theta) \\ (\cos\phi\sin\theta\cos\theta) & (\sin\phi(\cos^2\theta - \sin^2\theta)) \\ 0 & (2\cos\theta\sin\theta) \end{bmatrix}$$

and then the covariance in d is given by

$$\underset{(6\times6)}{\mathrm{cov}(d_i, d_j)} = \sum_k \sum_l \underset{(6\times2)}{e_{ik}}\ \underset{(2\times2)}{\mathrm{cov}(\psi_k, \psi_l)}\ \underset{(2\times6)}{e^T_{li}}$$

now suppose b such that it is composed of sums of elements of d, where the sum is over the data (ie individual unit vectors)

$$b = \left[\sum_{data} l^2, \sum_{data} lm, \sum_{data} ln, \sum_{data} m^2, \sum_{data} mn \sum_{data} n^2\right]$$

assuming that the data is completely uncorrellated,

$$\mathrm{cov}(b_i, b_j) = \sum_{data} \mathrm{cov}(d_i, d_j)$$

$$\operatorname{cov}(f_i^{(1)}, f_j^{(2)}) = \sum_k \sum_l \xi_{ik} \operatorname{cov}(b_k, b_l) \xi_{lj}^T$$

$$\underset{(3\times3)}{\operatorname{cov}(f_i^{(1)}, f_j^{(2)})} \quad \underset{(3\times6)}{\xi_{ik}} \quad \underset{(6\times6)}{\operatorname{cov}(b_k, b_l)} \quad \underset{(6\times3)}{\xi_{lj}^T}$$

f_i = unit vector of plane's normal = $[p^{(1)}, q^{(1)}, r^{(1)}]^T$

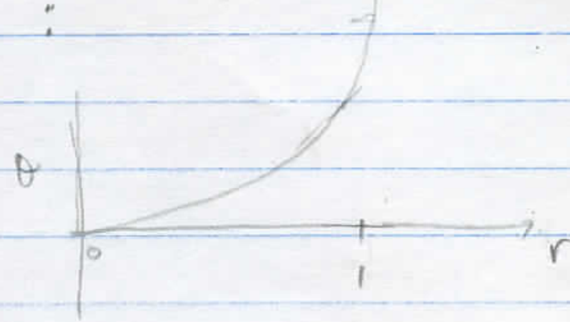
using perturbation theory for eigenvectors of sym. matrix:

$$\xi_{ik} = \left\{ \frac{f_i^{(2)}}{(\lambda_1-\lambda_2)} \alpha_k(2,1) + \frac{f_i^{(3)}}{(\lambda_1-\lambda_3)} \alpha_k(3,1) \right\}$$

$$\alpha_k(2,1) = \begin{bmatrix} (p^{(2)} p^{(1)}) \\ (p^{(2)} q^{(1)} + p^{(1)} q^{(2)}) \\ (p^{(2)} r^{(1)} + p^{(1)} r^{(2)}) \\ (q^{(1)} q^{(2)}) \\ (q^{(1)} r^{(2)} + r^{(1)} q^{(2)}) \\ (r^{(1)} r^{(2)}) \end{bmatrix} \qquad \alpha_k(3,1) = \begin{bmatrix} (p^{(3)} p^{(1)}) \\ (p^{(3)} q^{(1)} + p^{(1)} q^{(3)}) \\ (p^{(3)} r^{(1)} + p^{(1)} r^{(3)}) \\ (q^{(1)} q^{(3)}) \\ (q^{(1)} r^{(3)} + r^{(1)} q^{(3)}) \\ (r^{(1)} r^{(3)} \end{bmatrix}$$

Then suppose the plane's normal is given by $[\phi, \theta] = \underline{\Phi}$

then if $f = (p, q, r)$:



$$p = \cos\phi \cos\theta$$
$$q = \sin\phi \cos\theta$$
$$r = \sin\theta$$

$$\phi = \tan^{-1} q/p$$
$$\theta = \sin^{-1} r$$

in the vicinity of a point ϕ_0, θ_0

$$\phi \approx \tan^{-1}\frac{q_0}{p_0} - \frac{q_0}{p_0^2}\left(1 + \frac{q_0^2}{p_0^2}\right)^{-1}\delta p + \frac{1}{p_0}\left(1 + \frac{q_0^2}{p_0^2}\right)^{-1}\delta q$$

$$\theta \approx \sin^{-1} r_0 + (1 - r_0^2)^{-1/2}\,\delta r$$

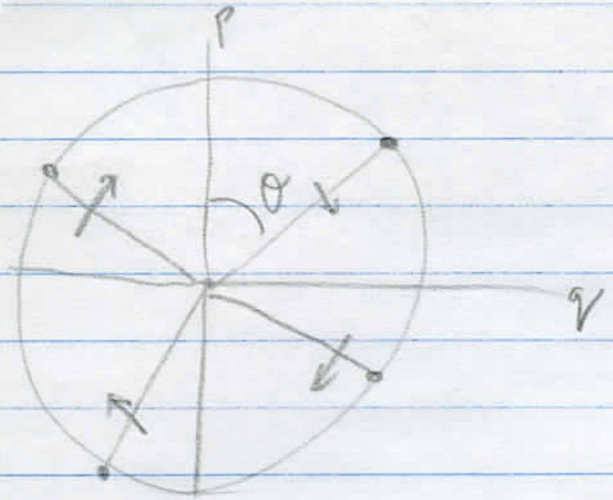
which allows us to write $\Phi_i \approx \Phi_i^0 + \sum_j t_{ij}\,\delta f_j$

$$t_{ij} = \begin{bmatrix} -\frac{q}{p^2}\left(1 + \frac{q^2}{p^2}\right)^{-1} & \frac{1}{p}\left(1 + \frac{q^2}{p^2}\right)^{-1} & 0 \\ 0 & 0 & (1 - r^2)^{-1/2} \end{bmatrix}$$

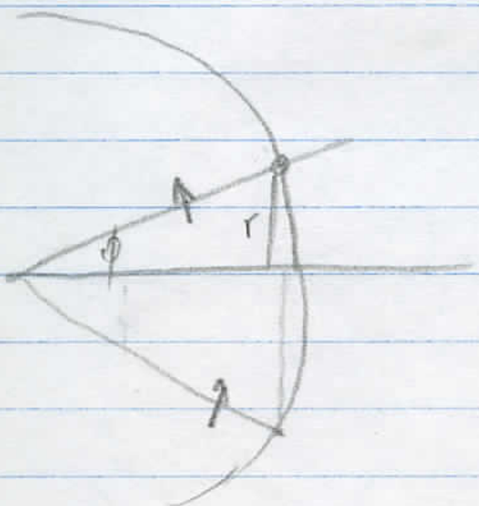
whence approximately the desired result :

$$\operatorname{cov}(\Phi_i, \Phi_j) = \sum_k \sum_l t_{ik}\,\operatorname{cov}(f_k, f_l)\,t^T_{lj}$$

(2x2) (2x3) (3x3) (3x2)



form works	$0 < \theta < 90^{\circ}$	$\delta\theta \propto -\delta p + \delta q$	$p+\ q+$
form works	$90 < \theta < 180$	$\delta\theta \propto -\delta p - \delta q$	$p-\ q+$
form works	$180 < \theta < 270$	$\delta\theta \propto +\delta p - \delta q$	$p-\ q-$
form works.	$270 < \theta < 360$	$\delta\theta \propto +\delta p + \delta q$	$p+\ q-$



$\phi = \sin^{-1}$

$0 < \phi < 90 \qquad \delta\phi = +\delta r \qquad r+$

$0 > \phi > -90 \qquad \delta\phi = -\delta r \qquad r-$