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 \( \phi_i \), the angle between the bedding pole and the plane of the great circle is called \( \psi_i \).

![Diagram of vector relationships]

2. If \( \hat{f} \) has components \( (P, q, r) \) (which are to be determined) and \( \hat{b}_i \) has components \( (d_i, m_i, n_i) \) (which are known, the data), vector analysis gives:

\[
\sin \psi_i = \cos \phi_i = \hat{f} \cdot \hat{b}_i = (d_i P + m_i q + n_i r)
\]

3. If the bedding pole was exactly on the plane of the great circle, then \( \phi_i = 90^\circ \) and \( \psi_i = 0^\circ \). But we expect scatter of the bedding poles, so we choose to find the components of \( \hat{f} \) which minimize:

\[
\text{ERROR} = E = \sum_i (\sin \psi_i)^2 = \sum_i (d_i P + m_i q + n_i r)^2
\]

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 unit 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 minimize $\text{Error} = E = \sum (p_i + q_i + r_i)^2$
subject to the constraint that $L = p^2 + q^2 + r^2 - 1 = 0$

6. This problem is conveniently solved by the method of Lagrange multipliers. This method defines an (as yet unknown) parameter $\lambda$. It 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:
\[
\begin{pmatrix}
\sum l_i^2 & \sum l_i q_i & \sum l_i r_i \\
\sum l_i q_i & \sum q_i^2 & \sum q_i r_i \\
\sum l_i r_i & \sum q_i r_i & \sum r_i^2
\end{pmatrix}
\begin{pmatrix}
p \\
q \\
r
\end{pmatrix}
= \lambda
\begin{pmatrix}
p \\
q \\
r
\end{pmatrix}
\]
\[
\text{or } M \mathbf{f} = \lambda \mathbf{f}
\]

8. The matrix equation is (7) is in the form of a standard eigenvalue–eigenvector equation well known to mathematicians. It has three solutions:
\[
\lambda_1, \begin{pmatrix} p_1 \\ q_1 \\ r_1 \end{pmatrix}, \lambda_2, \begin{pmatrix} p_2 \\ q_2 \\ r_2 \end{pmatrix}, \lambda_3, \begin{pmatrix} p_3 \\ q_3 \\ r_3 \end{pmatrix}
\]
One solution minimizes the error. One solution maximizes the error. One solution is an inflection point in the error. The solution with smallest $\lambda$ 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:

\[
E = \Sigma (p_{i} + q_{i} m_{i} + r_{i})^{2} = \Sigma \left(p^{2} l_{i}^{2} + q^{2} m_{i}^{2} + r^{2} n_{i}^{2} + 2pq \ell_{i} m_{i} + 2pr \ell_{i} n_{i} + 2qr m_{i} n_{i}\right) = p^{2} \Sigma l_{i}^{2} + q^{2} \Sigma m_{i}^{2} + r^{2} \Sigma n_{i}^{2} + 2pq \Sigma \ell_{i} m_{i} + 2pr \Sigma \ell_{i} n_{i} + 2qr \Sigma m_{i} n_{i}.
\]

Thus the error can be written as the matrix form:

\[
E = (p, q, r) \begin{pmatrix}
\Sigma l_{i}^{2} & \Sigma \ell_{i} m_{i} & \Sigma \ell_{i} n_{i} \\
\Sigma \ell_{i} m_{i} & \Sigma m_{i}^{2} & \Sigma m_{i} n_{i} \\
\Sigma \ell_{i} n_{i} & \Sigma m_{i} n_{i} & \Sigma n_{i}^{2}
\end{pmatrix} \begin{pmatrix}
p \\
q \\
r
\end{pmatrix}
\]

\[
= \hat{\lambda}^{T} M \hat{\lambda}
\]

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

\[
\text{Error} = E = \lambda
\]

so that \(\lambda\) has a simple, physical interpretation as the error on residual sum of squares.
Error analysis. Following assumptions made.

1. The errors in the measurement of the strike and dip $(\theta_i, \phi_i)$ of any single bedding plane are known (or can be conveniently estimated). This error is represented by the covariance matrix $\text{cov}(\theta_i, \phi_j)$. 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: $\text{cov}(\theta_i, \phi_j)$ find the covariance matrix of the bearing and plunge of the best fit plane's normal $(\mathbf{\pi})$, $\text{cov}(\mathbf{\pi}_i, \mathbf{\pi}_j)$

General procedure

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

   given some functions $f_j(x_j)$ where the $x_j$ are known only within some tolerance, say $\delta x_j$, then if we can write:
\[ \hat{f}_i(x_j) = f_i^0(x_j) + \sum_j \frac{\partial f_i}{\partial x_j} |_{x^0} \delta x_j \]
\[ = f_i^0(x_j) + \sum_j a_{ij} \delta x_j \]

Then approximately:

\[ \text{cov}(\hat{f}_i, \hat{f}_j) \approx \sum_k \sum_{i,k} a_{ik} \text{cov}(x_k, x_l) a_{jk} \]

**Specific Procedure**

1. Start with the covariance in the data \( \text{cov}(Y_i, Y_j) \)
2. Compute the covariance of the matrix of products of unit vector components (for one bedding plane) \( \text{cov}(d_{ij}, d_{kj}) \) by expanding the relations between the (bearing, plunge) data and the matrix elements. This relation is approx.

\[ d_i = d_i^0 + \sum E_{ij} \delta x_j \]

3. Recognize that since the data for different bedding planes is completely uncorrelated, the covariance of the matrix of sums of products is the sum of the covariances of the individual matrices.

\[ \text{cov}(b_i, b_j) = \sum_{\text{data}} \text{cov}(d_{ij}, d_{kj}) \]

4. Map the covariance of matrix elements into covariance of eigenvector (fold axis unit vector) components \( \text{cov}(f_i, f_j) \) using a perturbation expansion given by Wilkinson. The expansion leads to:

\[ \hat{f}_i = f_i^0 + \sum_k \delta f_k \]

5. Map the covariance in the unit vector into the covariance in the (bearing, plunge) = \( \hat{\Theta} \) of the fold axis by a Taylor series expansion of the contentious to polar transformations:

\[ \hat{\Theta}_i \approx \Theta_i^0 + \sum E_{ij} \delta f_j \]
Suppose data is a list of vectors $Y_i \equiv \{ \phi_i, \theta_i \}$ over data.

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

\[
(1, 2, 3) = (\text{NORTH}, \text{EAST}, \text{DOWN})
\]

\[
(\phi_i, \theta_i) = (\text{bearing\, not\,East,\, plunge})
\]

\[
\begin{align*}
  l &= \cos\phi \cos\theta \\
  m &= \sin\phi \cos\theta \\
  n &= \sin\theta
\end{align*}
\]

Circling around a point $(\phi_0, \theta_0)$ we have Taylor’s theorem:

\[
\begin{align*}
  l &= \cos \phi_0 \cos \theta_0 - \sin \phi_0 \cos \theta_0 \delta \phi - \cos \phi_0 \sin \theta_0 \delta \theta \\
  m &= \sin \phi_0 \cos \theta_0 + \cos \phi_0 \cos \theta_0 \delta \phi - \sin \phi_0 \sin \theta_0 \delta \theta \\
  n &= \sin \theta_0 + 0 + \sin \theta_0 \delta \theta
\end{align*}
\]

then suppose these are formed into products

\[
d = \begin{bmatrix} l^2, lm, ln, m^2, mn, n^2 \end{bmatrix}
\]

we can write then that:

\[
d_i = d_i^0 + \sum_{j=1}^{2} e_{ij} \delta Y_j
\]

where $e_{ij}$ is given by
\[ \mathbf{ij} = \begin{bmatrix} -2 \cos \phi \sin \phi \cos^2 \Theta & -2 \cos^2 \phi \cos \Theta \sin \Theta \\ (\cos^2 \phi - \sin^2 \phi) \cos^2 \Theta & -2 \cos \phi \sin \phi \cos \Theta \sin \Theta \\ -\sin \phi \cos \Theta \sin \Theta & (\cos \phi (\cos^2 \Theta - \sin^2 \Theta)) \\ (2 \cos \phi \sin \phi \cos \Theta) & (-2 \sin^2 \phi \cos \Theta \sin \Theta) \\ (\cos \phi \sin \phi \cos \Theta) & (\sin \phi (\cos^2 \Theta - \sin^2 \Theta)) \\ 0 & (2 \cos \Theta \sin \Theta) \end{bmatrix} \]

and then the covariance in \( d \) is given by

\[
\text{cov}(d_i, d_j) = \sum_{k} \sum_{l} \rho_{ik} \text{cov}(\psi_k, \psi_l) e_l^T e_k^T
\]

\((6 \times 6) \quad (6 \times 2) \quad (2 \times 2) \quad (2 \times 6)\)

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)

\[
b = \begin{bmatrix} \Sigma e^2_d & \Sigma e_m & \Sigma e_n & \Sigma m^2 & \Sigma mn & \Sigma n^2 \end{bmatrix}
\]

assuming that the data is completely uncorrelated,

\[
\text{cov}(b_i, b_j) = \Sigma \text{cov}(d_i, d_j)
\]

\(\text{data}\)
\[ \text{cov}(\mathbf{A}_i, \mathbf{A}_j) = \sum_{k} \sum_{x} \xi_{ik} \text{cov}(\mathbf{b}_k, \mathbf{b}_x) \xi_{kj}^T \]

\( (3 \times 3) \quad (3 \times 6) \quad (6 \times 6) \quad (6 \times 3) \)

\( \mathbf{f}_i \) = unit vector of plane's normal = \[ [p^{(0)}, q^{(0)}, r^{(0)}] \]

using perturbation theory for eigenvectors of sym. matrix:

\[ \xi_{ik} = \left\{ \frac{f_i^{(1)}}{(\lambda_1 - \lambda_2)} \mathbf{d}_k^{(2,1)} + \frac{f_i^{(3)}}{(\lambda_1 - \lambda_3)} \mathbf{d}_k^{(3,1)} \right\} \]

\[ \mathbf{d}_k^{(2,1)} = \begin{bmatrix} (p^{(0)}) & (p^{(1)}) \\ (p^{(2)}) & (p^{(0)} + p^{(1)} q^{(2)}) \\ (q^{(0)}) & (q^{(2)}) \\ (r^{(0)}) & (r^{(2)}) \end{bmatrix} \]

\[ \mathbf{d}_k^{(3,1)} = \begin{bmatrix} (p^{(0)}) & (p^{(1)}) & (p^{(2)}) & (p^{(3)}) \\ (p^{(1)}) & (p^{(0)}) & (p^{(3)}) & (p^{(2)}) \\ (q^{(0)}) & (q^{(1)}) & (q^{(2)}) & (q^{(3)}) \\ (r^{(0)}) & (r^{(1)}) & (r^{(2)}) & (r^{(3)}) \end{bmatrix} \]
Then suppose the plane's normal is given by $[\Phi, \Theta] = \Phi$

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

\[
p = \cos \Phi \cos \Theta \\
q = \sin \Phi \cos \Theta \\
r = \sin \Theta
\]

\[
\Phi = \tan^{-1} \frac{q}{p} \\
\Theta = \sin^{-1} r
\]

in the vicinity of a point $\Phi_0, \Theta_0$

\[
\Phi \approx \tan^{-1} \frac{\Phi_0}{P_0} - \frac{q_0}{p_0} \left( 1 + \frac{q_0^2}{p_0^2} \right)^{-1} \delta p + \frac{1}{P_0} \left( 1 + \frac{q_0^2}{p_0^2} \right)^{-1} \delta q \\
\Theta \approx \sin^{-1} \Theta_0 + (1 - r_0^2)^{-1/2} \delta r
\]

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

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

whence approximately the desired result:

\[
C(\Phi_i, \Phi_j) = \sum_k \sum_l t_{ik} \text{cov}(f_k, f_l) t_{lj}^T
\]

(2x2) (2x3) (3x3) (3x2)
For works $0 < \theta < 90^\circ$

\[
\begin{align*}
\phi &= \sin^{-1} \\
\theta &= \pi - \phi \\
\rho &= \phi \\
p &= \phi \\
q &= \phi
\end{align*}
\]

For works $90 < \theta < 180$

\[
\begin{align*}
\phi &= \sin^{-1} \\
\theta &= \pi - \phi \\
\rho &= \phi \\
p &= \phi \\
q &= \phi
\end{align*}
\]

For works $180 < \theta < 270$

\[
\begin{align*}
\phi &= \sin^{-1} \\
\theta &= \phi \\
\rho &= \phi \\
p &= \phi \\
q &= \phi
\end{align*}
\]

For works $270 < \theta < 360$

\[
\begin{align*}
\phi &= \sin^{-1} \\
\theta &= \phi \\
\rho &= \phi \\
p &= \phi \\
q &= \phi
\end{align*}
\]

\[
\begin{align*}
\phi &= \sin^{-1} \\
\theta &= \phi \\
\rho &= \phi \\
p &= \phi \\
q &= \phi
\end{align*}
\]