

1 Standard fit with multiple scattering

1.1 Fit with no material

Let us assume to have a series of plane measurements \vec{y}^* in locations x_1, x_2, \dots, x_n and a predictive model $y_i = y_i(\vec{\alpha}, x_i)$, where $\vec{\alpha}$ are parameters to be determined by fitting the measurements. The fit is performed minimizing the χ^2 :

$$\chi^2 = (\vec{y}(\vec{\alpha}) - \vec{y}^*)^t D^{-1} (\vec{y}(\vec{\alpha}) - \vec{y}^*) \quad (1)$$

where D is the digonal matrix containing the squared errors on the \vec{y}^* :

$$D = \begin{pmatrix} \sigma_1^2 & 0 & \dots & 0 \\ 0 & \sigma_2^2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \sigma_n^2 \end{pmatrix} \quad (2)$$

The minimization can be solved recursively by linearizing the prediction function:

$$\vec{y}(\vec{\alpha}) \simeq \vec{y}(\vec{\alpha}_0) + \frac{\partial \vec{y}}{\partial \vec{\alpha}} (\vec{\alpha} - \vec{\alpha}_0) = \vec{y}_0 + A \delta \vec{\alpha} \quad (3)$$

The derivative of the χ^2 is given by:

$$\frac{1}{2} \frac{\partial \chi^2}{\partial \vec{\alpha}} = A^t D^{-1} (A \delta \vec{\alpha} + \vec{y}_0 - \vec{y}^*) = 0 \quad (4)$$

that can be solved to give the parameters $\vec{\alpha}$:

$$\delta \vec{\alpha} = (A^t D^{-1} A)^{-1} A^t D^{-1} (\vec{y}^* - \vec{y}_0) \quad (5)$$

and the parameter covariance matrix, C :

$$\frac{1}{2} \frac{\partial^2 \chi^2}{\partial \vec{\alpha} \partial \vec{\alpha}} = C^{-1} = A^t D^{-1} A \quad (6)$$

1.2 Fit with material in front

Let us now assume that we have a layer of material before all the measurements at location $x_0 < x_i$, $i = 1, 2, \dots, n$ generating an average multiple scattering angle $\bar{\theta}$. We want to calculate how this affects the covariance matrix of the fit parameters.

Let $\vec{\alpha}$ be the parameters before the scattering layer and $\vec{\alpha}'$ those after the scattering layer toward the measurements. The following relation holds:

$$\vec{\alpha}' \simeq \vec{\alpha} + \frac{\partial \vec{\alpha}}{\partial \theta} \theta \quad (7)$$

This parameter variation affects the measurements:

$$\vec{y}' = \vec{y}(\vec{\alpha}') \simeq \vec{y}(\vec{\alpha}) + \frac{\partial \vec{y}}{\partial \vec{\alpha}} \frac{\partial \vec{\alpha}}{\partial \theta} \theta \quad (8)$$

and generates an additional component to the measurement covariance matrix, M :

$$M = \frac{\partial \vec{y}}{\partial \vec{\alpha}} \frac{\partial \vec{\alpha}}{\partial \theta} \bar{\theta}^2 \left(\frac{\partial \vec{y}}{\partial \vec{\alpha}} \frac{\partial \vec{\alpha}}{\partial \theta} \right)^t = A \frac{\partial \vec{\alpha}}{\partial \theta} \bar{\theta}^2 \left(\frac{\partial \vec{\alpha}}{\partial \theta} \right)^t A^t = \vec{u} \vec{u}^t \quad (9)$$

where the derivative of the parameters is taken at the scattering location x_0 and \vec{u} is given by:

$$\vec{u} = A \frac{\partial \vec{\alpha}}{\partial \theta} \bar{\theta} = A \vec{g} \bar{\theta} \quad (10)$$

The measurements error matrix becomes $S = D + M = D + \vec{u} \vec{u}^t$ and can be inverted using Miller's lemma:

$$S^{-1} = D^{-1} - \frac{D^{-1} \vec{u} \vec{u}^t D^{-1}}{1 + \vec{u}^t D^{-1} \vec{u}} \quad (11)$$

Replacing D^{-1} with S^{-1} in eq. (6) we obtain the updated covariance matrix:

$$C^{-1} = A^t S^{-1} A = A^t \left(D^{-1} - \frac{D^{-1} \vec{u} \vec{u}^t D^{-1}}{1 + \vec{u}^t D^{-1} \vec{u}} \right) A = A^t D^{-1} A - \frac{A^t D^{-1} \vec{u} \vec{u}^t D^{-1} A}{1 + \vec{u}^t D^{-1} D D^{-1} \vec{u}} \quad (12)$$

Letting C_0 be the covariance matrix obtained without the material in front we can rewrite eq. (12) as:

$$C^{-1} = C_0^{-1} - \frac{C_0^{-1} \vec{g} \bar{\theta}^2 \vec{g}^t C_0^{-1}}{1 + \vec{g}^t C_0^{-1} \vec{g} \bar{\theta}^2} = C_0^{-1} \left(C_0 - \frac{\vec{g} \vec{g}^t \bar{\theta}^2}{1 + \vec{g}^t C_0^{-1} \vec{g} \bar{\theta}^2} \right) C_0^{-1} \quad (13)$$

2 Kalman fit with multiple scattering

In the Kalman approach from outside in the covariance matrix of the parameters is obtained adding one measurement point at a time and finally adding the multiple scattering contribution from the scattering layer. The covariance matrix of the parameters is generated iteratively starting from a large external covariance matrix, C_{n+1} such that $C_{n+1}^{-1} = 0$. Using the notation where C_i is the covariance matrix after adding point x_i , we extract a recursive relation between the C_i by minizing the χ^2 :

$$\chi^2 = (\vec{\alpha}_i - \vec{\alpha}_{i+1})^t C_{i+1} (\vec{\alpha}_i - \vec{\alpha}_{i+1}) + \frac{(y_i(\vec{\alpha}_i) - y_i^*)^2}{\sigma_i^2} \quad (14)$$

where $\vec{\alpha}_{i+1}$ are the parameters determined in the previous iteration. The covariance of $\vec{\alpha}_i$ is given by:

$$C_i^{-1} = \frac{1}{2} \frac{\partial^2 \chi^2}{\partial \vec{\alpha}_i \partial \vec{\alpha}_i} = C_{i+1}^{-1} + \frac{1}{\sigma_i^2} \frac{\partial y_i}{\partial \vec{\alpha}_i} \left(\frac{\partial y_i}{\partial \vec{\alpha}_i} \right)^t \quad (15)$$

After adding all points starting from y_n and ending at y_1 , we have the covariance matrix before including the contribution from the multiple scattering:

$$C_1^{-1} = \sum_{i=1}^n \frac{1}{\sigma_i^2} \left(\frac{\partial y_i}{\partial \vec{\alpha}} \right)^t \frac{\partial y_i}{\partial \vec{\alpha}} \quad (16)$$

where we have dropped the index i in the parameters assuming to use always the most probable (true) value. We recall that:

$$A = \frac{\partial \vec{y}}{\partial \vec{\alpha}} = \begin{pmatrix} \frac{\partial y_1}{\partial \alpha_1} & \frac{\partial y_1}{\partial \alpha_2} & \dots & \frac{\partial y_1}{\partial \alpha_p} \\ \frac{\partial y_2}{\partial \alpha_1} & \frac{\partial y_2}{\partial \alpha_2} & \dots & \frac{\partial y_2}{\partial \alpha_p} \\ \dots & \dots & \dots & \dots \\ \frac{\partial y_n}{\partial \alpha_1} & \frac{\partial y_n}{\partial \alpha_2} & \dots & \frac{\partial y_n}{\partial \alpha_p} \end{pmatrix} = \begin{pmatrix} \frac{\partial y_1}{\partial \vec{\alpha}} \\ \frac{\partial y_2}{\partial \vec{\alpha}} \\ \dots \\ \frac{\partial y_n}{\partial \vec{\alpha}} \end{pmatrix} \quad (17)$$

therefore:

$$C_1^{-1} = \sum_{i=1}^n \frac{1}{\sigma_i^2} \left(\frac{\partial y_i}{\partial \vec{\alpha}} \right)^t \frac{\partial y_i}{\partial \vec{\alpha}} = \sum_{i,j=1}^n \left(\frac{\partial y_i}{\partial \vec{\alpha}} \right)^t \frac{\delta_{ij}}{\sigma_i^2} \frac{\partial y_j}{\partial \vec{\alpha}} = A^t D^{-1} A = C_0^{-1} \quad (18)$$

We now add the contribution from the scattering layer:

$$C = C_0 + \frac{\partial \vec{\alpha}}{\partial \theta} \bar{\theta}^2 \left(\frac{\partial \vec{\alpha}}{\partial \theta} \right)^t = C_0 + \vec{g} \vec{g}^t \bar{\theta}^2 = (A^t D^{-1} A)^{-1} + \vec{v} \vec{v}^t \quad \text{where } \vec{v} = \frac{\partial \vec{\alpha}}{\partial \theta} \bar{\theta} \quad (19)$$

The inverse of the covariance matrix is then given by:

$$C^{-1} = A^t D^{-1} A - \frac{A^t D^{-1} A \vec{v} \vec{v}^t A^t D^{-1} A}{1 + \vec{v}^t A^t D^{-1} D D^{-1} A \vec{v}} \quad (20)$$

but since $\vec{u} = A \vec{v}$, the above equation becomes:

$$C^{-1} = A^t D^{-1} A - \frac{A^t D^{-1} \vec{u} \vec{u}^t D^{-1} A}{1 + \vec{u}^t D^{-1} D D^{-1} \vec{u}} \quad (21)$$

that is identical to eq. (12). It is thus demonstrated that the global and Kalman approaches are equivalent.

3 Discussion of the multiple scattering terms

We now calculate the derivative of the parameters with respect to the MS angle in the simplified situation when $D = 0$. We note that:

$$\frac{\partial \vec{\alpha}}{\partial \theta} = \frac{\partial \vec{\alpha}}{\partial \vec{p}} \frac{\partial \vec{p}}{\partial \theta} \quad (22)$$

so we start with the derivative of the parameters with respect to the momentum.

Derivative of D :

$$D = \frac{1}{a}(T - p_\perp), \text{ so: } \frac{\partial D}{\partial \vec{p}} = \frac{1}{a} \left(\frac{\partial T}{\partial \vec{p}} - \frac{\partial p_\perp}{\partial \vec{p}} \right) \quad (23)$$

where

$$T = \sqrt{p_\perp^2 - 2a(xp_y - yp_x) + a^2(x^2 + y^2)} \quad (24)$$

leading to:

$$\frac{\partial D}{\partial \vec{p}} = \frac{1}{a} \left(\frac{p_x + ay}{T} - \frac{p_x}{p_\perp}, \frac{p_y - ax}{T} - \frac{p_y}{p_\perp}, 0 \right) \quad (25)$$

since however $D = 0$ then $T = p_\perp$ the derivative simplifies into:

$$\frac{\partial D}{\partial \vec{p}} = \frac{1}{p_\perp} (y, -x, 0) \quad (26)$$

Derivative of φ_0 :

Recalling that:

$$\cos \varphi_0 = \frac{p_x + ay}{T} = \frac{p_x + ay}{p_\perp} \text{ and } \tan \varphi_0 = \frac{p_y - ax}{p_x + ay} \quad (27)$$

we get that:

$$\frac{\partial \varphi_0}{\partial \vec{p}} = \frac{\cos^2 \varphi_0}{p_x + ay} (-\tan \varphi_0, 1, 0) = \frac{(p_x + ay)^2}{(p_x + ay)p_\perp^2} \left(-\frac{p_y - ax}{p_x + ay}, 1, 0 \right) \quad (28)$$

that simplifies into:

$$\frac{\partial \varphi_0}{\partial \vec{p}} = \frac{1}{p_\perp^2} (-p_y + ax, p_x + ay, 0) = \frac{1}{p_\perp} (-\sin \varphi_0, \cos \varphi_0, 0) \quad (29)$$

Derivative of C :

the derivative of the half curvature $C = a/(2p_\perp)$ is:

$$\frac{\partial C}{\partial \vec{p}} = \frac{a}{2} \left(-\frac{p_x}{p_\perp^3}, -\frac{p_y}{p_\perp^3}, 0 \right) = \frac{a}{2p_\perp^3} (-p_x, -p_y, 0) = \frac{C}{p_\perp^2} (-p_x, -p_y, 0) \quad (30)$$

Derivative of $\lambda = \cot \theta$:

the derivative of $\lambda = p_z/p_\perp$ is:

$$\frac{\partial \lambda}{\partial \vec{p}} = \left(-\frac{p_x p_z}{p_\perp^3}, -\frac{p_y p_z}{p_\perp^3}, \frac{1}{p_\perp} \right) = \frac{1}{p_\perp} \left(-\frac{p_x p_z}{p_\perp^2}, -\frac{p_y p_z}{p_\perp^2}, 1 \right) \quad (31)$$

Derivative of z_0 :

Recall that $z_0 = z - \lambda s/(2C) = z - p_z s/a$, where s is the phase and that $s = \tan^{-1}(p_y/p_x) - \varphi_0$ then:

$$\frac{\partial z_0}{\partial \vec{p}} = \left(\frac{p_z}{a} \left(\frac{p_y}{p_\perp^2} + \frac{\partial \varphi_0}{\partial p_x} \right), \frac{p_z}{a} \left(-\frac{p_x}{p_\perp^2} + \frac{\partial \varphi_0}{\partial p_y} \right), -s/a \right) = \left(\frac{p_z}{a} \frac{ax}{p_\perp^2}, \frac{p_z}{a} \frac{ay}{p_\perp^2}, -s/a \right) \quad (32)$$

that simplifies to:

$$\frac{\partial z_0}{\partial \vec{p}} = \left(\frac{\lambda x}{p_\perp}, \frac{\lambda y}{p_\perp}, -s/a \right) \quad (33)$$

Summing everything up:

$$\frac{\partial \vec{\alpha}}{\partial \vec{p}} = \begin{pmatrix} \frac{y}{p_\perp} & -\frac{x}{p_\perp} & 0 \\ -\frac{\sin \varphi_0}{p_\perp} & \frac{\cos \varphi_0}{p_\perp} & 0 \\ -\frac{C p_x}{p_\perp^2} & -\frac{C p_y}{p_\perp^2} & 0 \\ -\frac{p_x p_z}{p_\perp^3} & -\frac{p_y p_z}{p_\perp^3} & \frac{1}{p_\perp} \\ \frac{\lambda x}{p_\perp} & \frac{\lambda y}{p_\perp} & -s/a \end{pmatrix} = \frac{1}{p_\perp} \begin{pmatrix} y & -x & 0 \\ -\sin \varphi_0 & \cos \varphi_0 & 0 \\ -C p_x & -C p_y & 0 \\ -\frac{p_x p_z}{p_\perp^2} & -\frac{p_y p_z}{p_\perp^2} & 1 \\ \lambda x & \lambda y & -\frac{s}{2C} \end{pmatrix} \quad (34)$$

The full derivative relative to the transverse multiple scattering angle is then given by:

Transverse

$$\frac{\partial \vec{\alpha}}{\partial \theta} = \frac{\partial \vec{\alpha}}{\partial \vec{p}} \frac{\partial \vec{p}}{\partial \theta} = \frac{p}{p_{\perp}^2} \begin{pmatrix} y & -x & 0 \\ -\sin \varphi_0 & \cos \varphi_0 & 0 \\ -\frac{C p_x}{p_{\perp}} & -\frac{C p_y}{p_{\perp}} & 0 \\ -\frac{p_x p_z}{p_{\perp}^2} & -\frac{p_y p_z}{p_{\perp}^2} & 1 \\ \lambda x & \lambda y & -\frac{s}{2C} \end{pmatrix} \begin{pmatrix} -p_y \\ p_x \\ 0 \end{pmatrix} = \frac{p}{p_{\perp}^2} \begin{pmatrix} -(x p_x + y p_y) \\ p_x \cos \varphi_0 + p_y \sin \varphi_0 \\ 0 \\ 0 \\ \lambda(y p_x - x p_y) \end{pmatrix} \quad (35)$$

This can be simplified taking into account the parametric helix equation as a function of the phase s :

$$\frac{\partial \vec{\alpha}}{\partial \theta} = \frac{p}{p_{\perp}} \begin{pmatrix} -\frac{1}{2C} \sin s \\ \cos s \\ 0 \\ 0 \\ \frac{1}{2C} (\cos s - 1) \end{pmatrix} \quad (36)$$

where we remind that

$$s = 2 \sin^{-1} \left(C \sqrt{\frac{r^2 - D^2}{1 + 2CD}} \right) = \sin^{-1} [2C(x \cos \varphi_0 + y \sin \varphi_0)] \quad (37)$$

when $D = 0$ then:

$$rC = \sin \frac{s}{2} \quad (38)$$

In order to estimate the MS effect on an $R\varphi$ measurement at a radius R one has to estimate the derivative of $R\varphi$ with respect to the helix parameters:

$$y = R\varphi = R\varphi_0 + R \sin^{-1} \left(\frac{RC + (1 + CD)D/R}{1 + 2CD} \right) = R\varphi_0 + R \sin^{-1} A \quad (39)$$

then

D derivative

$$\frac{\partial y}{\partial D} = \frac{R}{\sqrt{1 - A^2}} \frac{(1 + 2CD)^2/R - 2C[RC + (1 + CD)D/R]}{(1 + 2CD)^2} \quad (40)$$

that becomes for $D = 0$:

$$\frac{\partial y}{\partial D} = \frac{1}{\sqrt{1 - R^2 C^2}} (1 - 2R^2 C^2) \quad (41)$$

If we let t be the phase at radius R then:

$$\frac{\partial y}{\partial D} = \frac{1 - 2\sin^2 \frac{t}{2}}{\cos \frac{t}{2}} = \frac{\cos t}{\cos \frac{t}{2}} = 2\cos \frac{t}{2} - \frac{1}{\cos \frac{t}{2}} \simeq 1 \quad (42)$$

The φ_0 **derivative** is easy $\partial y / \partial \varphi_0 = R = \sin(t/2)/C$. Finally the

C derivative:

$$\frac{\partial y}{\partial C} = \frac{R}{\sqrt{1 - A^2}} \frac{(R + D^2/R)(1 + 2CD) - 2D(RC + (1 + CD)D/R)}{(1 + 2CD)^2} \quad (43)$$

that becomes for $D = 0$:

$$\frac{\partial y}{\partial C} = \frac{R^2}{\sqrt{1 - R^2 C^2}} = \frac{\sin^2 \frac{t}{2}}{C^2 \cos \frac{t}{2}} \quad (44)$$

Finally, setting to t the phase at the measurement layer and s at the scattering layer, the MS effect is given by:

$$\frac{\delta R\varphi}{\theta} = \left[\frac{\partial R\varphi}{\partial \vec{\alpha}} \right]_{\omega=t} \left[\frac{\partial \vec{\alpha}}{\partial \theta} \right]_{\omega=s} = \frac{\sin \frac{t}{2}}{C} \cos s - \frac{1}{2C} \sin s \frac{\cos t}{\cos \frac{t}{2}} \simeq \frac{t - s}{2C} \quad (45)$$