The quantity to be minimized is

$$D = \sum_{hkl} w_{hkl}[F_o - F_c(x,y,z)]^2$$

For each individual hkl reflection, the three derivatives with respect to x, y and z are set equal to 0:

$$\frac{1}{2}\frac{\partial D}{\partial x} = w_{hkl}[F_o - F_c(x,y,z)]\frac{\partial F_c}{\partial x} = 0$$

$$\frac{1}{2}\frac{\partial D}{\partial y} = w_{hkl}[F_o - F_c(x,y,z)]\frac{\partial F_c}{\partial y} = 0$$

$$\frac{1}{2}\frac{\partial D}{\partial z} = w_{hkl}[F_o - F_c(x,y,z)]\frac{\partial F_c}{\partial z} = 0$$

where $F_c(x,y,z)$ is the desired calculated structure factor. If each F_c is approximated by a truncated Taylor series (neglecting second and higher powers):

$$F_c(x,y,z) = F_c(x_0,y_0,z_0) + \frac{\partial F_c(x_0,y_0,z_0)}{\partial x}\Delta x + \frac{\partial F_c(x_0,y_0,z_0)}{\partial y}\Delta y + \frac{\partial F_c(x_0,y_0,z_0)}{\partial z}\Delta z$$

where (x_0,y_0,z_0) are the initial parameters, e.g.,from the initial structure solution and $(\Delta x, \Delta y, \Delta z)$ are the parameter shifts needed to improve the agreement between F_o and F_c. In the following, $F_c(x_0,y_0,z_0)$ is abbreviated as F_c.

Thus, for each hkl reflection,

$$\frac{\partial D}{\partial x} = w_{hkl}\left[F_o - F_c - \frac{\partial F_c}{\partial x}\Delta x - \frac{\partial F_c}{\partial y}\Delta y - \frac{\partial F_c}{\partial z}\Delta z\right]\frac{\partial F_c}{\partial x} = 0$$

$$\frac{\partial D}{\partial y} = w_{hkl}\left[F_o - F_c - \frac{\partial F_c}{\partial x}\Delta x - \frac{\partial F_c}{\partial y}\Delta y - \frac{\partial F_c}{\partial z}\Delta z\right]\frac{\partial F_c}{\partial y} = 0$$

$$\frac{\partial D}{\partial z} = w_{hkl}\left[F_o - F_c - \frac{\partial F_c}{\partial x}\Delta x - \frac{\partial F_c}{\partial y}\Delta y - \frac{\partial F_c}{\partial z}\Delta z\right]\frac{\partial F_c}{\partial z} = 0$$

and, identifying F_o-F_c as ΔF:

$$\frac{\partial D}{\partial x} = w_{hkl}\Delta F\frac{\partial F_c}{\partial x} - w_{hkl}\frac{\partial F_c}{\partial x}\frac{\partial F_c}{\partial x}\Delta x - w_{hkl}\frac{\partial F_c}{\partial y}\frac{\partial F_c}{\partial x}\Delta y - w_{hkl}\frac{\partial F_c}{\partial z}\frac{\partial F_c}{\partial x}\Delta z = 0$$

$$\frac{\partial D}{\partial y} = w_{hkl}\Delta F\frac{\partial F_c}{\partial y} - w_{hkl}\frac{\partial F_c}{\partial x}\frac{\partial F_c}{\partial y}\Delta x - w_{hkl}\frac{\partial F_c}{\partial y}\frac{\partial F_c}{\partial y}\Delta y - w_{hkl}\frac{\partial F_c}{\partial z}\frac{\partial F_c}{\partial y}\Delta z = 0$$

$$\frac{\partial D}{\partial z} = w_{hkl}\Delta F\frac{\partial F_c}{\partial z} - w_{hkl}\frac{\partial F_c}{\partial x}\frac{\partial F_c}{\partial z}\Delta x - w_{hkl}\frac{\partial F_c}{\partial y}\frac{\partial F_c}{\partial z}\Delta y - w_{hkl}\frac{\partial F_c}{\partial z}\frac{\partial F_c}{\partial z}\Delta z = 0$$

If the derivatives are summed over, e.g., four reflections (labelling ΔF, F_c and w_{hkl} as ΔF_i, F_i and w_i, where i is the reflection number), the following equations are obtained:

$$w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial x}\Delta x+w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial y}\Delta y+w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial z}\Delta z+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial x}\Delta x+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial y}\Delta y+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial z}\Delta z+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial x}\Delta x+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial y}\Delta y+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial z}\Delta z+w_4\frac{\partial F_4}{\partial x}\frac{\partial F_4}{\partial x}\Delta x+w_4\frac{\partial F_4}{\partial x}\frac{\partial F_4}{\partial y}\Delta y+w_4\frac{\partial F_4}{\partial x}\frac{\partial F_4}{\partial z}\Delta z=w_1\Delta F_1\frac{\partial F_1}{\partial x}+w_2\Delta F_2\frac{\partial F_2}{\partial x}+w_3\Delta F_3\frac{\partial F_3}{\partial x}+w_4\Delta F_4\frac{\partial F_4}{\partial x}$$

$$w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial y}\Delta x+w_1\frac{\partial F_1}{\partial y}\frac{\partial F_1}{\partial y}\Delta y+w_1\frac{\partial F_1}{\partial y}\frac{\partial F_1}{\partial z}\Delta z+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial y}\Delta x+w_2\frac{\partial F_2}{\partial y}\frac{\partial F_2}{\partial y}\Delta y+w_2\frac{\partial F_2}{\partial y}\frac{\partial F_2}{\partial z}\Delta z+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial y}\Delta x+w_3\frac{\partial F_3}{\partial y}\frac{\partial F_3}{\partial y}\Delta y+w_3\frac{\partial F_3}{\partial y}\frac{\partial F_3}{\partial z}\Delta z+w_4\frac{\partial F_4}{\partial x}\frac{\partial F_4}{\partial y}\Delta x+w_4\frac{\partial F_4}{\partial y}\frac{\partial F_4}{\partial y}\Delta y+w_4\frac{\partial F_4}{\partial y}\frac{\partial F_4}{\partial z}\Delta z=w_1\Delta F_1\frac{\partial F_1}{\partial y}+w_2\Delta F_2\frac{\partial F_2}{\partial y}+w_3\Delta F_3\frac{\partial F_3}{\partial y}+w_4\Delta F_4\frac{\partial F_4}{\partial y}$$

$$w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial z}\Delta x+w_1\frac{\partial F_1}{\partial y}\frac{\partial F_1}{\partial z}\Delta y+w_1\frac{\partial F_1}{\partial z}\frac{\partial F_1}{\partial z}\Delta z+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial z}\Delta x+w_2\frac{\partial F_2}{\partial y}\frac{\partial F_2}{\partial z}\Delta y+w_2\frac{\partial F_2}{\partial z}\frac{\partial F_2}{\partial z}\Delta z+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial z}\Delta x+w_3\frac{\partial F_3}{\partial y}\frac{\partial F_3}{\partial z}\Delta y+w_3\frac{\partial F_3}{\partial z}\frac{\partial F_3}{\partial z}\Delta z+w_4\frac{\partial F_4}{\partial x}\frac{\partial F_4}{\partial z}\Delta x+w_4\frac{\partial F_4}{\partial y}\frac{\partial F_4}{\partial z}\Delta y+w_4\frac{\partial F_4}{\partial z}\frac{\partial F_4}{\partial z}\Delta z=w_1\Delta F_1\frac{\partial F_1}{\partial z}+w_2\Delta F_2\frac{\partial F_2}{\partial z}+w_3\Delta F_3\frac{\partial F_3}{\partial z}+w_4\Delta F_4\frac{\partial F_4}{\partial z}$$

These are the three normal equations, one for each adjustable parameter. Collecting common terms and rearranging,

$$\left(w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial x}+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial x}+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial x}+w_4\frac{\partial F_4}{\partial x}\frac{\partial F_4}{\partial x}\right)\Delta x+\left(w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial y}+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial y}+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial y}+w_4\frac{\partial F_4}{\partial x}\frac{\partial F_4}{\partial y}\right)\Delta y+\left(w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial z}+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial z}+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial z}+w_4\frac{\partial F_4}{\partial x}\frac{\partial F_4}{\partial x}\right)\Delta z=w_1\Delta F_1\frac{\partial F_1}{\partial x}+w_2\Delta F_2\frac{\partial F_2}{\partial x}+w_3\Delta F_3\frac{\partial F_3}{\partial x}+w_4\Delta F_4\frac{\partial F_4}{\partial x}$$

$$\left(w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial y}+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial y}+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial y}+w_4\frac{\partial F_4}{\partial x}\frac{\partial F_4}{\partial y}\right)\Delta x+\left(w_1\frac{\partial F_1}{\partial y}\frac{\partial F_1}{\partial y}+w_2\frac{\partial F_2}{\partial y}\frac{\partial F_2}{\partial y}+w_3\frac{\partial F_3}{\partial y}\frac{\partial F_3}{\partial y}+w_4\frac{\partial F_4}{\partial y}\frac{\partial F_4}{\partial y}\right)\Delta y+\left(w_1\frac{\partial F_1}{\partial y}\frac{\partial F_1}{\partial z}+w_2\frac{\partial F_2}{\partial y}\frac{\partial F_2}{\partial z}+w_3\frac{\partial F_3}{\partial y}\frac{\partial F_3}{\partial z}+w_4\frac{\partial F_4}{\partial y}\frac{\partial F_4}{\partial x}\right)\Delta z=w_1\Delta F_1\frac{\partial F_1}{\partial y}+w_2\Delta F_2\frac{\partial F_2}{\partial y}+w_3\Delta F_3\frac{\partial F_3}{\partial y}+w_4\Delta F_4\frac{\partial F_4}{\partial y}$$

$$\left(w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial z}+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial z}+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial z}+w_4\frac{\partial F_4}{\partial y}\frac{\partial F_4}{\partial z}\right)\Delta x+\left(w_1\frac{\partial F_1}{\partial y}\frac{\partial F_1}{\partial z}+w_2\frac{\partial F_2}{\partial y}\frac{\partial F_2}{\partial z}+w_3\frac{\partial F_3}{\partial y}\frac{\partial F_3}{\partial z}+w_4\frac{\partial F_4}{\partial y}\frac{\partial F_4}{\partial z}\right)\Delta y+\left(w_1\frac{\partial F_1}{\partial z}\frac{\partial F_1}{\partial z}+w_2\frac{\partial F_2}{\partial z}\frac{\partial F_2}{\partial z}+w_3\frac{\partial F_3}{\partial z}\frac{\partial F_3}{\partial z}+w_4\frac{\partial F_4}{\partial z}\frac{\partial F_4}{\partial x}\right)\Delta z=w_1\Delta F_1\frac{\partial F_1}{\partial z}+w_2\Delta F_2\frac{\partial F_2}{\partial z}+w_3\Delta F_3\frac{\partial F_3}{\partial z}+w_4\Delta F_4\frac{\partial F_4}{\partial z}$$

These equations can be represented in matrix notation:

$$\begin{pmatrix} w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial x}+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial x}+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial x}+w_4\frac{\partial F_4}{\partial x}\frac{\partial F_4}{\partial x} & w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial y}+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial y}+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial y}+w_4\frac{\partial F_4}{\partial x}\frac{\partial F_4}{\partial y} & w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial z}+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial z}+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial z}+w_4\frac{\partial F_4}{\partial x}\frac{\partial F_4}{\partial x} \\ w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial y}+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial y}+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial y}+w_4\frac{\partial F_4}{\partial x}\frac{\partial F_4}{\partial y} & w_1\frac{\partial F_1}{\partial y}\frac{\partial F_1}{\partial y}+w_2\frac{\partial F_2}{\partial y}\frac{\partial F_2}{\partial y}+w_3\frac{\partial F_3}{\partial y}\frac{\partial F_3}{\partial y}+w_4\frac{\partial F_4}{\partial y}\frac{\partial F_4}{\partial y} & w_1\frac{\partial F_1}{\partial y}\frac{\partial F_1}{\partial z}+w_2\frac{\partial F_2}{\partial y}\frac{\partial F_2}{\partial z}+w_3\frac{\partial F_3}{\partial y}\frac{\partial F_3}{\partial z}+w_4\frac{\partial F_4}{\partial y}\frac{\partial F_4}{\partial x} \\ w_1\frac{\partial F_1}{\partial x}\frac{\partial F_1}{\partial z}+w_2\frac{\partial F_2}{\partial x}\frac{\partial F_2}{\partial z}+w_3\frac{\partial F_3}{\partial x}\frac{\partial F_3}{\partial z}+w_4\frac{\partial F_4}{\partial y}\frac{\partial F_4}{\partial z} & w_1\frac{\partial F_1}{\partial y}\frac{\partial F_1}{\partial z}+w_2\frac{\partial F_2}{\partial y}\frac{\partial F_2}{\partial z}+w_3\frac{\partial F_3}{\partial y}\frac{\partial F_3}{\partial z}+w_4\frac{\partial F_4}{\partial y}\frac{\partial F_4}{\partial z} & w_1\frac{\partial F_1}{\partial z}\frac{\partial F_1}{\partial z}+w_2\frac{\partial F_2}{\partial z}\frac{\partial F_2}{\partial z}+w_3\frac{\partial F_3}{\partial z}\frac{\partial F_3}{\partial z}+w_4\frac{\partial F_4}{\partial z}\frac{\partial F_4}{\partial x} \end{pmatrix} = \begin{pmatrix}\Delta x\\ \Delta y\\ \Delta z\end{pmatrix}\begin{pmatrix} w_1\Delta F_1\frac{\partial F_1}{\partial x}+w_2\Delta F_2\frac{\partial F_2}{\partial x}+w_3\Delta F_3\frac{\partial F_3}{\partial x}+w_4\Delta F_4\frac{\partial F_4}{\partial x} \\ w_1\Delta F_1\frac{\partial F_1}{\partial y}+w_2\Delta F_2\frac{\partial F_2}{\partial y}+w_3\Delta F_3\frac{\partial F_3}{\partial y}+w_4\Delta F_4\frac{\partial F_4}{\partial y} \\ w_1\Delta F_1\frac{\partial F_1}{\partial z}+w_2\Delta F_2\frac{\partial F_2}{\partial z}+w_3\Delta F_3\frac{\partial F_3}{\partial z}+w_4\Delta F_4\frac{\partial F_4}{\partial z} \end{pmatrix}$$

or, in shorthand notation, as:

$$\begin{pmatrix} a_{11}\ a_{12}\cdots a_{1m} \\ a_{21}\ a_{22}\cdots a_{2m} \\ \vdots \\ a_{m1}\ a_{m1}\cdots a_{mm} \end{pmatrix}\begin{pmatrix}\Delta x_1\\ \Delta x_2\\ \vdots\\ \Delta x_m\end{pmatrix}=\begin{pmatrix}b_1\\ b_2\\ \vdots\\ b_m\end{pmatrix}\quad \text{or}\quad [A]\,\Delta x=b$$

where the elements of the **A** and **b** matrices are

$$a_{ij}=\sum_{hkl} w_{hkl}\frac{\partial F_c}{\partial x_i}\frac{\partial F_c}{\partial x_j} \qquad\qquad b_i=\sum_{hkl} w_{hkl}\Delta F_c\frac{\partial F_c}{\partial x_i}$$