IV.A.3. Iteration Scheme

The linearity hypothesis, that is, the assumption that the Taylor expansion of the theoretical values around the prior expectation value truncates after the linear term, is in general only approximately true. Therefore, the parameter values $\overline{P}'$ resulting from application of Bayes' equations are also only approximately correct. To obtain more accurate values, the Taylor expansion, Eq. (IV A.4), may be performed not around $\overline{P}$ but around the new (intermediate) values $\overline{P}^{(n)}$, where *n* represents the *n*th iteration and $\overline{P}^{(0)} = \overline{P}$. That is, we assume

$$\begin{aligned} T &\cong \overline{T}^{(n)} + G^{(n)}\left(P - \overline{P}^{(n)}\right) = \overline{T}^{(n)} + G^{(n)}\left(P - \overline{P}^{(0)} + \overline{P}^{(0)} - \overline{P}^{(n)}\right) \\ &= \overline{T}^{(n)} + G^{(n)}\left(\overline{P}^{(0)} - \overline{P}^{(n)}\right) + G^{(n)}\left(P - \overline{P}^{(0)}\right) \end{aligned} \qquad \text{(IV A3.1)}$$

Here the sensitivity matrix $G^{(n)}$ and the theoretical values $\overline{T}^{(n)}$ are evaluated at $P = \overline{P}^{(n)}$. With Eq. (IV A3.1) for *T*, the formula analogous to Eq. (IV A.13) is

$$\begin{aligned} \exp\Bigg[-\frac{1}{2}\Bigg\{ & \left(P - \overline{P}^{(0)}\right)^t \left[\left(M^{(n+1)}\right)^{-1} - \left(M^{-1} + G^{(n)t} V^{-1} G^{(n)}\right)\right]\left(P - \overline{P}^{(0)}\right) \\ & + \left(P - \overline{P}^{(0)}\right)^t \Bigg[\left(M^{(n+1)}\right)^{-1}\left(\overline{P}^{(0)} - \overline{P}^{(n+1)}\right) \\ & \qquad - G^{(n)t} V^{-1}\left(D - \overline{T}^{(n)} - G^{(n)}\left(\overline{P}^{(0)} - \overline{P}^{(n)}\right)\right)\Bigg] \\ & + \Bigg[\left(\overline{P}^{(0)} - \overline{P}^{(n+1)}\right)^t \left(M^{(n+1)}\right)^{-1} \\ & \qquad - \left(D - \overline{T}^{(n)} - G^{(n)}\left(\overline{P}^{(0)} - \overline{P}^{(n)}\right)\right)^t V^{-1} G^{(n)}\Bigg]\left(P - \overline{P}^{(0)}\right) \\ & + \left(\overline{P}^{0} - \overline{P}^{(n+1)}\right)^t \left(M^{(n+1)}\right)^{-1}\left(\overline{P}^{(0)} - \overline{P}^{(n+1)}\right) \\ & - \left(D - \overline{T}^{(n)} - G^{(n)}\left(\overline{P}^{(0)} - \overline{P}^{(n)}\right)\right)^t V^{-1}\left(D - \overline{T}^{(n)} - G^{(n)}\left(\overline{P}^{(0)} - \overline{P}^{(n)}\right)\right)\Bigg\}\Bigg] \end{aligned} \qquad \text{(IV A3.2)}$$

= constant .

The iterative forms of Bayes' equations follow immediately, by replacing *G* by $G^{(n)}$ and *T* by $T^{(n)} - G^{(n)}\left(P^{(0)} - P^{(n)}\right)$ in the equations of Section IV A.1. Note that again we have dropped the bars to simplify the notation.

Explicitly, the equations are as follows: For the M+W version, Eq. (IV A1.3) becomes

$$\begin{aligned} M^{(n+1)} &= \left(M^{-1} + W^{(n)}\right)^{-1} \qquad & P^{(n+1)} &= P^{(0)} + M^{(n+1)} Y^{(n)} \\ W^{(n)} &= G^{(n)t} V^{-1} G^{(n)} \qquad & Y^{(n)} &= G^{(n)t} V^{-1}\left(D - T^{(n)} - G^{(n)}\left(P^{(0)} - P^{(n)}\right)\right) \end{aligned} \quad . \qquad \text{(IV A3.3)}$$

For the I+Q version, the covariance equations, Eqs. (IV A1.5) and (IV A1.6), take the form

$$Q^{(n)} = G^{(n)t} V^{-1} G^{(n)} M \qquad \text{and} \qquad M^{(n+1)} = M\left(I + Q^{(n)}\right)^{-1} \quad , \qquad \text{(IV A3.4)}$$

and for the N+V version, Eqs. (IV A1.10) and (IV A1.13) become

$$M^{(n+1)} = M - M\,G^{(n)t}\left(N^{(n)} + V\right)^{-1} G^{(n)} M \quad \text{with} \quad N = G^{(n)} M\, G^{(n)t} \quad . \qquad \text{(IV A3.5)}$$

For all versions, the parameter equation is

$$P^{(n+1)} = P^{(0)} + M^{(n+1)}\, G^{(n)\,t}\, V^{-1}\left(D - T^{(n)} - G^{(n)}\left(P^{(0)} - P^{(n)}\right)\right) \quad . \qquad \text{(IV A3.6)}$$

To control the number of iterations

When running SAMMY, the default number of iterations is 2; that is, SAMMY stops after calculating $P^{(2)}$ and $M^{(2)}$. This value was chosen based on early experience which suggested that, for many practical applications, little was gained from additional iterations: After two iterations, the value of a parameter would generally be accurate to within the uncertainty on that parameter. To illustrate, suppose the "true" value of a parameter was 1.23456789 ± 0.03456789. After two iterations, the value was found to be approximately 1.23500000 ± 0.03500000, so no useful new information is gained by continuing the computations.

Nevertheless, especially during early stages of an analysis, the user will often find it helpful to iterate more times. To increase the number of iterations, specify ITMAX in columns 46–50 of line 2 (i.e., card set 2) of the INPut file, Table VIA.1.

Caveat: Setting ITMAX = 0 in the INPut file will cause the default value ITMAX = 2 to be used. In order to obtain zero iterations (i.e., to evaluate the cross section but not update the parameter values), the user must specify "DO NOT SOLVE BAYES Equations" in the command section of the INPut file.

Caveat: Some older compilers interpret "1" (one) in column 49 as "10" (ten). To avoid undue difficulties caused by having misplaced a number by one column, SAMMY assumes that a value of ITMAX greater than 9 was an input error. If more than 9 iterations are wanted, the user must insert the negative of the correct value into the INPut file.

At present there are no criteria in SAMMY for stopping the iterations when convergence is reached. These may be added in the future.