IV.A.1. Derivation of SAMMY's Solution Schemes

Three distinct versions of Bayes' equations are used in the SAMMY computer code. More specifically, it is the equation for M' that differs in the three versions. Each has computational advantages and disadvantages for particular situations; these are described in Section IV.B. In this section, the three versions are derived from the forms found in Eqs. (IV A.16) and (IV A.17), which are repeated here:

$$\left(M'\right)^{-1} = M^{-1} + G^t V^{-1} G \tag{IV A1.1}$$

and

$$P' = P + M' G^t V^{-1} \left(D - T\right) \quad . \tag{IV A1.2}$$

Here the bars have been dropped for simplicity of notation.

For readers who may be unfamiliar with matrix notation, the final equations are given at the end of this section with indices and summations explicitly displayed.

M+W Version

The version of Bayes' Equations which uses Eqs. (IV A1.1) and (IV A1.2) directly is denoted the "M+W" version,

$$\begin{aligned} M' &= \left(M^{-1} + W\right)^{-1} & \qquad P' &= P + M'Y \\ W &= G^t V^{-1} G & \qquad Y &= G^t V^{-1} \left(D - T\right) \quad , \end{aligned} \tag{IV A1.3}$$

in which the matrix quantities Y and W have been introduced to simplify later discussion. (See especially Section IV.E.1.)

In this form, the relationship of Bayes' equations to the more common least-squares equations is transparent: If the prior parameter covariance matrix M is infinite on the diagonal $\left(M^{-1} = 0\right)$, then the equations in Eq. (IV A1.3) become the least-squares equations; the only difference is in the first equation. Hence the least-squares equations may be considered to be a special case of Bayes' equations; alternatively, Bayes' Equations may be viewed as generalized least squares.

I+Q Version

Multiplying Eq. (IV A1.1) on the right by M and on the left by M' gives

$$\begin{aligned}(M')^{-1} M &= M^{-1}M + G^t V^{-1} G M = I + G^t V^{-1} G M \\ M'(M')^{-1} M &= M = M'\left(I + G^t V^{-1} G M\right) \quad .\end{aligned} \qquad \text{(IV A1.4)}$$

Defining Q via

$$Q = G^t V^{-1} G M \qquad \text{(IV A1.5)}$$

puts Eq. (IV A1.4) into the form

$$M' = M\left(I + Q\right)^{-1} \quad . \qquad \text{(IV A1.6)}$$

Substituting Eq. (IV A1.6) into Eq. (IV A1.2) gives

$$P' = P + M\left(I + Q\right)^{-1} G^t V^{-1}\left(D - T\right) \quad , \qquad \text{(IV A1.7)}$$

which is Bayes' equation for P' in the I+Q version.

N+V Version

To obtain the N+V version of Bayes' equations, use the identity

$$X^{-1} = Z\left(XZ\right)^{-1} \qquad \text{(IV A1.8)}$$

$$\text{with} \quad X = I + Q \quad \text{and} \quad Z = G^t\left(G M G^t + V\right)^{-1} G \quad . \qquad \text{(IV A1.9)}$$

Combining Eqs. (IV A1.6) with Eqs. (IV A1.8) and (IV A1.9) gives

$$M' = M G^t\left(G M G^t + V\right)^{-1} G\left\{\left(I + Q\right) G^t\left(G M G^t + V\right)^{-1} G\right\}^{-1} \quad , \qquad \text{(IV A1.10)}$$

which can be simplified by defining

$$N = G M G^t \qquad \text{(IV A1.11)}$$

to give

$$\begin{aligned}M' &= M G^t\left(N + V\right)^{-1} G\left\{\left(I + G^t V^{-1} G M\right) G^t\left(N + V\right)^{-1} G\right\}^{-1} \\ &= M G^t\left(N + V\right)^{-1} G\left\{G^t\left(N + V\right)^{-1} G + G^t V^{-1} G M G^t\left(N + V\right)^{-1} G\right\}^{-1} \qquad \text{(IV A1.12)} \\ &= M G^t\left(N + V\right)^{-1} G\left\{G^t\left(N + V\right)^{-1} G + G^t V^{-1} N\left(N + V\right)^{-1} G\right\}^{-1} \quad .\end{aligned}$$

Rearranging gives

$$
\begin{aligned}
M' &= M\,G^t\left(N+V\right)^{-1}G\left\{G^t\left(\left(N+V\right)^{-1}+V^{-1}N\left(N+V\right)^{-1}\right)G\right\}^{-1} \\
&= M\,G^t\left(N+V\right)^{-1}G\left\{G^t\left(\left(N+V\right)^{-1}+V^{-1}\left(N+V-V\right)\left(N+V\right)^{-1}\right)G\right\}^{-1} \\
&= M\,G^t\left(N+V\right)^{-1}G\left\{G^t\left(\left(N+V\right)^{-1}+V^{-1}-\left(N+V\right)^{-1}\right)G\right\}^{-1} \\
&= M\,G^t\left(N+V\right)^{-1}G\left\{G^tV^{-1}G\right\}^{-1} \\
&= M\,G^t\left(N+V\right)^{-1}V\,V^{-1}G\left\{G^tV^{-1}G\right\}^{-1} \\
&= M\,G^t\left(N+V\right)^{-1}\left(N+V-N\right)V^{-1}G\left\{G^tV^{-1}G\right\}^{-1} \\
&= M\,G^t\left(\left[I-\left(N+V\right)^{-1}N\right]V^{-1}G\right)\left\{G^tV^{-1}G\right\}^{-1} \\
&= M\,G^t\left(V^{-1}G-\left(N+V\right)^{-1}G\,M\,G^t\,V^{-1}G\right)\left\{G^tV^{-1}G\right\}^{-1} \\
&= M\left(G^t\,V^{-1}G-G^t\left(N+V\right)^{-1}G\,M\,G^t\,V^{-1}G\right)\left\{G^tV^{-1}G\right\}^{-1} \\
&= M-M\,G^t\left(N+V\right)^{-1}G\,M \quad . \qquad \text{(IV A1.13)}
\end{aligned}
$$

This is the N+V version of Bayes' Equation for M':

$$
M' = M - M\,G^t\left(N+V\right)^{-1}G\,M \quad . \qquad \text{(IV A1.14)}
$$

The N+V version of Bayes' equation for P' is found by inserting Eq. (IV A1.14) into Eq. (IV A1.2) and rearranging:

$$
\begin{aligned}
P' &= P+\left[M-M\,G^t\left(N+V\right)^{-1}G\,M\right]G^t\,V^{-1}\left(D-T\right) \\
&= P+\left[M\,G^t-M\,G^t\left(N+V\right)^{-1}G\,MG^t\right]V^{-1}\left(D-T\right) \\
&= P+M\,G^t\left[I-\left(N+V\right)^{-1}N\right]V^{-1}\left(D-T\right) \\
&= P+M\,G^t\left[I-\left(N+V\right)^{-1}\left[N+V-V\right]\right]V^{-1}\left(D-T\right) \qquad \text{(IV A1.15)} \\
&= P+M\,G^t\left[I-\left(N+V\right)^{-1}\left(N+V\right)+\left(N+V\right)^{-1}V\right]V^{-1}\left(D-T\right) \\
&= P+M\,G^t\left[I-I+\left(N+V\right)^{-1}V\right]V^{-1}\left(D-T\right) \\
&= P+M\,G^t\left(N+V\right)^{-1}\left(D-T\right) \quad .
\end{aligned}
$$

Equations with indices and summations explicitly displayed:

M+W Version, Eq. (IV A1.3):

$$M'_{ij} = \left(M^{-1} + W\right)^{-1}_{ij} \qquad P_i' = P_i + \sum_j M_{ij}' \, Y_j$$
$$W_{ij} = \sum_{km} G_{ki} V^{-1}_{km} G_{mj} \qquad Y_j = \sum_{km} G_{kj} \, V^{-1}_{km} \left(D_m - T_m\right) \tag{IV A1.16}$$

I+Q Version, Eqs.(IV A1.5), (IV A1.6), and (IV A1.7):

$$\begin{aligned} Q_{ij} &= \sum_{kmn} G_{ki} \, V^{-1}_{km} G_{mn} M_{nj} \\ M'_{ij} &= \sum_k M_{ik} \left(I + Q\right)^{-1}_{kj} \\ P_i' &= P_i + \sum_{jkm} M'_{ij} G_{kj} V^{-1}_{km} \left(D_m - T_m\right) \end{aligned} \tag{IV A1.17}$$

N+V Version, Eqs. (IV A1.11), (IV A1.14), and (IV A1.15):

$$\begin{aligned} N_{km} &= \sum_{ij} G_{ki} M_{ij} G_{mj} \\ M'_{ij} &= M_{ij} - \sum_{nklm} M_{in} G_{kn} \left(N + V\right)^{-1}_{kl} G_{lm} M_{mj} \\ P'_i &= P_i + \sum_{nkl} M_{in} G^t{}_{kn} \left(N + V\right)^{-1}_{kl} \left(D_l - T_l\right) \end{aligned} \tag{IV A1.18}$$