IV.A.2. Chi-Squared and Weighted Residuals

The negative of the constant term (the *P*-independent term) in the exponent of Eq. (IVA.13), which we shall label as χ^2_{Bayes} and denote the "Bayesian chi squared," is of the form

$$\chi^2_{\text{Bayes}} = -\left(\bar{P}-\bar{P}'\right)^t \left(M'\right)^{-1} \left(\bar{P}-\bar{P}'\right) + \left(D-\bar{T}\right)^t V^{-1} \left(D-\bar{T}\right) \quad . \tag{IV A2.1}$$

The second term in this expression is exactly the usual χ^2 value, defined as

$$\chi^2_{\text{LS}} = \left(D-\bar{T}\right)^t V^{-1} \left(D-\bar{T}\right) \quad . \tag{IV A2.2}$$

The least-squares χ^2 is always larger than the Bayesian χ^2 because the difference [the first term in the right-hand side of Eq.(IV A2.1)] is the negative of a squared quantity. What is observed during a successful Bayes fit is that the value of the least-squares χ^2_{LS} decreases with each iteration, while the value of the Bayesian χ^2_{Bayes} changes very little. In fact, the value of χ^2_{LS} becomes very close to the value of χ^2_{Bayes} as the iterations proceed. (See Section IV.A.3 for a discussion of iteration as compensation for nonlinearity.)

Hence, the Bayesian χ^2 is, in some sense, a measure of the "best fit" that can be found between this theoretical formulation and these experimental data. When a very small χ^2_{LS} value is considered to be a goal of the analysis process, but the value of χ^2_{Bayes} is relatively large, the analyst may find it prudent to look for problems with either the theory or the data before attempting to find a good fit. For example, spin assignments might be incorrect (Section II.C.1), background might not have been properly included (Section III.E.3.a), or multiple-scattering corrections might be needed (Section III.D).

The expression for χ^2_{Bayes} can be written in terms of known quantities as follows: Replacing $\left(\bar{P}-\bar{P}'\right)$ by its value as given in the expression in Eq. (IV.A.16) gives

$$\begin{aligned}
\chi^2_{\text{Bayes}} &= -\left(\bar{P}-\bar{P}'\right)^t \left(M'\right)^{-1} \left(\bar{P}-\bar{P}'\right) + \left(D-\bar{T}\right)^t V^{-1} \left(D-\bar{T}\right) \\
&= -\left(\left(D-T\right)^t V^{-1} G M'\right) \left(M'\right)^{-1} \left(M' G^t V^{-1} \left(D-T\right)\right) + \left(D-\bar{T}\right)^t V^{-1} \left(D-\bar{T}\right) \\
&= -\left(D-T\right)^t V^{-1} G M' G^t V^{-1} \left(D-T\right) + \left(D-\bar{T}\right)^t V^{-1} \left(D-\bar{T}\right) \\
&= \left(D-\bar{T}\right)^t \left\{-V^{-1} G M' G^t V^{-1} + V^{-1}\right\} \left(D-\bar{T}\right) \quad .
\end{aligned} \tag{IV A2.3}$$

In the M+W version for M', χ^2_{Bayes} therefore becomes

$$\chi^2_{\text{Bayes}} = \left(D-\bar{T}\right)^t \left\{-V^{-1}G\left(M^{-1}+W\right)^{-1} G^t\, V^{-1} + V^{-1}\right\}\left(D-\bar{T}\right) \quad , \qquad \text{(IV A2.4)}$$

where W is again defined as $G^t\, V^{-1}\, G$.

In the I+Q version, χ^2_{Bayes} takes the form

$$\chi^2_{\text{Bayes}} = \left(D-\bar{T}\right)^t \left\{-V^{-1}G\,M\left(I+Q\right)^{-1} G^t\, V^{-1} + V^{-1}\right\}\left(D-\bar{T}\right) \quad , \qquad \text{(IV A2.5)}$$

where Q is $G^t\, V^{-1}\, G\, M$.

Finally, in the N+V version,

$$\chi^2_{\text{Bayes}} = \left(D-\bar{T}\right)^t \left\{-V^{-1}G\left[M - M\,G^t\left(N+V\right)^{-1} G\,M\right]G^t\, V^{-1} + V^{-1}\right\}\left(D-\bar{T}\right), \qquad \text{(IV A2.6)}$$

in which N is equal to $G\,M\,G^t$. The expression in the curly brackets in Eq. (IV A2.6) can be simplified significantly as

$$\begin{aligned}
\{\ \} &= -V^{-1}G\left[M - M\,G^t\left(N+V\right)^{-1} G\,M\right]G^t\,V^{-1} + V^{-1} \\
&= -V^{-1}G\,M\,G^t\,V^{-1} + V^{-1}G\,M\,G^t\left(N+V\right)^{-1} G\,M\,G^t\,V^{-1} + V^{-1} \\
&= -V^{-1}N\,V^{-1} + V^{-1}N\left(N+V\right)^{-1} N\,V^{-1} + V^{-1} \\
&= V^{-1}\left[-N + N\left(N+V\right)^{-1} N + V\right]V^{-1} \\
&= V^{-1}\left[-N + \left(N+V-V\right)\left(N+V\right)^{-1} N + V\right]V^{-1} \qquad \text{(IV A2.7)} \\
&= V^{-1}\left[-N + N - V\left(N+V\right)^{-1} N + V\right]V^{-1} \\
&= V^{-1}\left[-V\left(N+V\right)^{-1}\left(N+V-V\right) + V\right]V^{-1} \\
&= V^{-1}\left[-V + V\left(N+V\right)^{-1} V + V\right]V^{-1} \\
&= V^{-1}\left[V\left(N+V\right)^{-1} V\right]V^{-1} \quad = \quad \left(N+V\right)^{-1} \quad .
\end{aligned}$$

Making this substitution into Eq. (IV A2.6) gives

$$\chi^2_{\text{Bayes}} = \left(D-\bar{T}\right)^t \left(N+V\right)^{-1}\left(D-\bar{T}\right) \qquad \text{(IV A2.8)}$$

for the N+V version of χ^2_{Bayes}.

Values for χ^2 (of both types) are reported in the SAMMY output file SAMMY.LPT (see Section VII.A). It should be noted, however, that SAMMY does not report $\chi^2/$ *dof* (where *dof* = degrees of freedom = NDAT − NPAR, with NDAT being the number of data points and NPAR the number of varied parameters), since with Bayes' method *dof* can be zero or negative. Instead SAMMY will report χ^2 and χ^2/NDAT.

Caveat: In the past (prior to the release of sammy-7.0.0 in 2006), the value of χ^2_{LS}, as reported in the SAMMY.LPT file, was calculated under the implicit assumption that the data covariance matrix V was diagonal. This is no longer true; χ^2_{LS} is now calculated using the actual data covariance matrix, including off-diagonal elements if they are present.

Another quantity that the analyst will often find useful to examine is the so-called weighted residual, which is the difference between measured value and theoretical value weighted (divided) by the uncertainty on the measured value. Specifically, the weighted residual at point i is defined as

$$R_i^{\mathrm{LS}} = \left(D_i - T_i\right) \Big/ \sqrt{V_{ii}} \quad , \qquad \text{(IV A2.9)}$$

a formula that implicitly assumes that the data covariance matrix is diagonal, since off-diagonal elements are ignored. To ask for this array to be printed, the user should specify "PRINT WEIGHTED RESIDuals" in the command section of the INPut file; see Table VI A1.2. The array will be printed, however, only if the data covariance matrix is diagonal.

SAMMY recognizes another array related to the weight residuals and denotes it as the "Bayesian weighted residual,"

$$R_i^{\mathrm{B}} = \sum_j \left(N + V\right)_{ij}^{-1} \left(D_j - T_j\right) \quad . \qquad \text{(IV A2.10)}$$

No particular physical interpretation is applied to this quantity. To calculate and print this array, insert the command "PRINT BAYES WEIGHTED residuals" into the INPut file. If the command "PRINT WEIGHTED RESIDuals" is given, and this array is generated in the normal course of solving Bayes' equations, then it will be printed even though it was not explicitly called for.