III.E.3.b. User-supplied data-reduction parameters

When uncertainties inherent in the parameters of the data-reduction process are carefully propagated through that process, the covariance matrix associated with the reduced data is off-diagonal. While SAMMY can handle off-diagonal data covariance matrices, it is often more convenient as well as more informative to treat the data covariance matrix as diagonal and incorporate the uncertainty information directly into the solution of Bayes' equations.

To understand how this is done, let d represent the raw (unreduced) data and D the reduced data. The relationship between D and d is

$$D_i = f_i\left(\{d\},\{q\}\right) \quad , \qquad \text{(III E3 b.1)}$$

where f_i is some function of $\{d\}$ (which represents the entire set of raw data) and of $\{q\}$ (which represents the set of data-reduction parameters). A small increment in D may then be written as

$$\delta D_i = \sum_j \frac{\partial f_i}{\partial d_j} \delta d_j + \sum_k \frac{\partial f_i}{\partial q_k} \delta q_k \quad . \qquad \text{(III E3 b.2)}$$

Squaring this expression, taking expectation values, and noting that the d_j and q_k are mutually independent give

$$\left\langle \delta D_i \; \delta D_{i'} \right\rangle = \sum_j \frac{\partial f_i}{\partial d_j} \Delta^2 d_j \frac{\partial f_{i'}}{\partial d_j} + \sum_{k,k'} \frac{\partial f_i}{\partial q_k} \left\langle \delta q_k \; \delta q_{k'} \right\rangle \frac{\partial f_{i'}}{\partial q_{k'}} \qquad \text{(III E3 b.3)}$$

for the covariance between D_i and $D_{i'}$. In Eq. (III E3 b.3), use has been made of the uncorrelated nature of the raw data:

$$\left\langle \delta d_j \, \delta d_{j'} \right\rangle = \Delta^2 d_j \; \delta_{j\,j'} \quad . \qquad \text{(III E3 b.4)}$$

The first term in Eq. (III E3 b.3) represents the statistical uncertainty on D_i. Generally, it is diagonal with respect to i and i', since f_i will usually depend only on d_i and not on other $d_{i'}$, but we have included off-diagonal terms for the sake of completeness. The second term contains information from the data-reduction process. Generally, this term is off-diagonal with respect to i and i'; that is, the reduced data D_i all depend upon the same parameters q_k, and thus are correlated. Thus the data covariance matrix $V_{i\,i'}$ to be used in Bayes' equations involves off-diagonal terms.

It is possible for the full covariance matrix to be calculated from Eq. (III E3 b.3) and read directly into SAMMY (see Section VI.C.2). However, all data points that are connected by off-diagonal terms need to be included in the same analysis. Because typical time-of-flight experiments may involve thousands of data points, this process is often impractical computationally.

An alternative method of handling uncertainties on data-reduction parameters is to treat those parameters as variables whose value is to be determined by the analysis process, that is, to treat them in the same fashion as the resonance parameters.

In the development of Bayes' equations (Section IV), the conditional probability $p(D|PX)$ was needed. Since the data-reduction parameters $\{q\}$ are now considered to be a part of the set $\{P\}$, Eq. (IV A1.3) requires the probability of D being true given that $\{q\}$ are exactly the correct values. That is, we use the data covariance matrix V formed from only the first term in Eq. (III E3 b.3), the second term giving zero if the values for $\{q\}$ are exact.

Since data D, as well as theory T, now depend on parameters P, Eq. (II A1.4) must be expanded to include

$$T(P) - D(q) = \overline{T} - \overline{D} + G\left(P - \overline{P}\right) - g\left(q - \overline{q}\right) \quad , \qquad \text{(III E3 b.5)}$$

in which we have set the partial derivative of D_i with respect to q_k equal to g_{ik}; that is,

$$\frac{\partial D_i}{\partial q_k} = g_{ik} \quad . \qquad \text{(III E3 b.6)}$$

Therefore, by expanding the set of parameters $\{P\}$ to include the data-reduction parameters $\{q\}$, and by redefining G_{ik}, the partial derivative of the theory T_i with respect to the parameter P_k, to be the partial derivative of $(T_i - D_i)$ with respect to P_k, the equations take on the exact form discussed in Section IV.A.

To use this method in SAMMY, the analyst must generate the partial derivatives g_{ik} prior to the SAMMY runs, and provide the values to SAMMY. (The code ALEX [DL83 and NL84] may be used for this purpose.) Input details are given in Section VI.C of this report.

Caveat: This option has been available in SAMMY almost from the beginning, but it has (to the author's knowledge) never been used extensively and hence never been thoroughly tested. Moreover, the techniques used are not optimal. Unless there is demand for this option, it will probably be discontinued with the next release of the code.