IV.E.3. Least Squares and Other Extensions of SAMMY's Methodology

The least-squares method can be considered as a special case of Bayes' equations, in which the initial parameter covariance matrix (PCM) M is diagonal and infinite (so that the inverse M^{-1} is zero). Nonetheless, in practice it is not easy to reach that limit when creating input for SAMMY. The usual technique is to provide a very large prior uncertainty for each parameter, large enough to be "effectively infinite." Using this technique, however, can lead to numerical problems. In particular, large prior uncertainties on resonance energies will often permit two resonances to interchange positions – an untenable feature.

To circumvent this difficulty and to facilitate comparisons with other codes that do assume a diagonal and infinite prior PCM, several options have been added to SAMMY. The relevant test case is tr163; the procedure is outlined below.

Step a. For each of the data sets, generate Y_i and W_i as described in the previous section. The command line

```
GENERATE Y AND W MATrices      or     YW
```

must be in the input file for each run.

Step b. Fit the data sets using the M+W scheme, including the following commands in the INPut file:

```
USE LEAST SQUARES TO give pcm for initial parameters
REMEMBER ORIGINAL PArameter values
READ Y AND W MATRICEs         or       WY
```

The first of these directs SAMMY to assume that the inverse of the prior covariance matrix is zero; this command is optional (though required if one wishes to do least squares). The second command causes a file REMORI.PAR to be created; this file contains values for $P^{(0)}$ and M^{-1}, as needed in the iterative form of Bayes' equations for M+W [Eq. (IV A3.3)]. The third command is always needed when invoking the M+W method in the resolved resonance region.

If values of starting parameters are not extremely close to the "true" results, there may be divergence problems. In that case, it may also be necessary to include the command

```
TAKE BABY STEPS WITH least squares method
```

in the INPut file. This command will cause the change in the parameter increment $(P'-P)$ to be 1/10 the calculated value of $M'Y$ [see Eq. (IV A3.1) or Eq. (IV B3.1)], and will often alleviate the divergence problems.

Step c. For each data set, generate a new Y_i and W_i using the parameter values determined in step b. Include these command lines

```
GENERATE Y AND W MATrices   or     YW
USE REMEMBERED ORIGInal parameter values
```

The second of these lines does not tell SAMMY to calculate theoretical cross sections at the original parameter values but rather to use $P^{(0)}$, as specified in the REMORI.PAR file, for generating Y via the iterative form of Bayes' equations [Eq. (IV A3.3)]. That file (with that name) must be available in the subdirectory in which these runs are made.

Step d. Fit the data sets using the M+W scheme, with the commands

```
USE REMEMBERED ORIGInal parameter values
READ Y AND W MATRICEs    or       WY
```

The "use remembered . . ." command will cause SAMMY to use the $P^{(0)}$ and M^{-1} from REMORI.PAR when solving for updated parameter values and covariance matrix, as in Eq. (IV A3.3). Again, it may be necessary to include the "take baby steps . . ." command.

Step e. Repeat steps c and d, as many times as desired, or until convergence (i.e., until there are no more changes in the χ^2 values for any of the data sets).

Test case tr163 has been set up to repeat steps c and d twice more (steps e and f, h and i). In addition, two command files (test163_many and test163hi) allow the user to rerun steps h and i 20 more times, each time overwriting the previous results (to avoid keeping so many intermediate files) while keeping track of the changes in the χ^2 values.

These options were implemented by the author to facilitate intercomparisons among three R-matrix codes (SAMMY, EDA [GH75], and RAC [CZ95]), as part of an IAEA Cooperative Research Project on Light-Element Standards [AC05, INDC02, INDC03, INDC04,VP04].