

### IV.E.1. Simultaneous Fitting to Several Data Sets

The M+W scheme can be used for truly simultaneous fitting to several independent data sets in the resolved-resonance region. Any number of data sets of any type (capture, fission, integral, transmission, etc.) may be included. The procedure requires a series of separate SAMMY runs, first to generate the information separately for each data set and then to solve Bayes' Equations once for the entire system. The procedure is as follows:

**Step a.** Create a single PARAmeter file containing only R-matrix parameters and no measurement-specific information. Flag all variables of interest; PUP no parameters. This parameter file will be used as the prior parameter set for all runs in steps b through d below.

**Step b.** For each independent data set, create an INPut file as usual. Put all measurement-related information into the INPut file (see the end of Table VI A.1); PUP parameters as needed (Section IV.D.2). Include the command

GENERATE Y AND W MATrices      *or*      YW

in the INPut file. Run SAMMY with this INPut file, the PARAmeter file from step a, and the appropriate DATa file. SAMMY will produce sub-matrices  $Y_i$  and  $W_i$ , which are this data set's contribution to  $Y$  and  $W$  needed in Bayes' Equations (Section IV.B.3). Arrays  $Y_i$  and  $W_i$  are defined as

$$Y_i = G_i^T V_i^{-1} (D - T_i) \quad \text{and} \quad W_i = G_i^T V_i^{-1} G_i, \quad (\text{IV E1.1})$$

in which the subscript  $i$  denotes the specific data set. These values are stored in file SAMMY.YWY, which the user should rename and keep for use in step d.

**Step c.** Repeat step b as many times as needed, once for each data set.

**Step d.** Once  $Y_i$  and  $W_i$  are known for each set of experimental data, they can be summed over the data sets  $i$ , giving

$$Y = \sum_i Y_i \quad \text{and} \quad W = \sum_i W_i. \quad (\text{IV E1.2})$$

These matrices will be used in Bayes' equations, Eq. (IV B3.2) and Eq. (IV B3.4), respectively, to solve for updated parameter values and covariance matrix. This step is accomplished by an additional SAMMY run in which the INPut file includes the phrase

READ Y AND W MATRICES      *or*      WY

The PARAmeter file from step a is used, and a dummy name may be given for the data set. Names of the files containing the sub-matrices  $Y_i$  and  $W_i$  are specified, one per line, immediately following the dummy data-file name in the input stream.

This run produces the SAMMY.PAR and SAMMY.COV files. Be sure to rename these to use in later steps.

If iteration for nonlinearities is to be used, an additional command is required in the INPut file in step d:

REMEMBER ORIGINAL Parameter values

This 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)].

Step e. To iterate for nonlinearities, create a second INPut file for each data set identical to the INPut file created in step b but containing one additional command:

USE REMEMBERED ORIGINAL parameter values

This command 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.

Run SAMMY with this INPut file and the appropriate data file, using the PARAmeter file and COVariance matrix created in step d. This will cause SAMMY to generate a new  $Y_i$  and  $W_i$  using the parameter values determined in Step b.

Step f. Repeat step e as many times as needed, once for each data set.

Step g. Fit the data sets using the M+W scheme using 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).

Step h. Repeat steps e, f, and g as many times as desired, or until convergence (i.e., until there are no more changes in the  $\chi^2$  values for any of the data sets).

Step i. To obtain plot files with the final fits to the data, it is necessary to make another set of runs, one for each data set. In these runs, the INPut files should include the command

GENERATE PLOT FILE Automatically

Test cases tr082, tr089, tr131, and tr149 give examples of steps a through d of this procedure. A slight variation of this procedure is used for least-squares runs in test case tr163; see Section IV.E.3 for details.