Use of Covariance Matrices in SAMMY

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Like all R-matrix codes with which this author is familiar, SAMMY[1] makes use of some form of least-squares equations for determining the parameter values that provide the best fit of experiment to theory. However, the direction of development of the fitting procedure is somewhat different from conventional treatments. In this paper, a description will be given of the derivation and implementation of the many options available in the SAMMY code. Simple examples will be used to illustrate the usefulness of these options.

Implementation of the fitting procedure in SAMMY involves the use of Bayes' equations, which can be viewed as "generalized least squares."[2] Three different but equivalent forms of Bayes' equations are available in SAMMY, each being more efficient for particular applications. Each involves the use of a data covariance matrix (DCM), which is a first-order mathematical description of the interrelationships between the individual members of the experimental data set; these interrelationships arise from data-reduction processes such as normalization. Until recently, most R-matrix analyses implicitly assumed that the DCM was diagonal; a few analyses included off-diagonal components due to normalization and/or background corrections to the data.

The option to include the fully off-diagonal DCM has always been available in SAMMY, but the inherit limitations of that procedure (the sheer size of the array) made it impractical to use very often. Several years ago, this author recognized that the mathematical form of the DCM would permit symbolically inverting the matrix, eliminating the necessity to generate, store, or explicitly invert the large matrix. This implicit data covariance (IDC) procedure has been implemented into the SAMMY code and has been shown to be far more efficient (with respect to both computer time and computer memory) and more accurate than the explicit treatment. [3,4]

A second improvement in the treatment of uncertainties in SAMMY is the ability to propagate uncertainties on nonvaried parameters (denoted "propagated uncertainty parameters,"

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[1] *Updated Users' Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations*, N. M. Larson, ENDF-364 and ORNL/TM-9179/R6, Oak Ridge National Laboratory, Oak Ridge, TN (May 2003). Also ORNL/TM-9179/R7, to be published in 2006.

[2] The one difference between Bayes' equations and conventional least squares is the additional assumption implicit in least squares: the prior parameter covariance matrix is infinite and diagonal. While the least-squares assumption can be used for fitting in SAMMY, it is not necessary to use this restrictive assumption.

[3] "Treatment of Data Uncertainties," N. M. Larson, ND2004 (*International Conference on Nuclear Data for Science and Technology*, Sept. 26–Oct. 1, 2004), page 374 *ff*.

[4] "On the Efficient Treatment of Data Covariance Matrices," N. M. Larson, *71st Annual Meeting of the Southeastern Section of the APS, Oak Ridge, TN,* November 11–13, 2004.

or PUPs). The PUP method provides identical results (to first order) to fitting raw data while varying the parameter; this has been demonstrated both algebraically and numerically.[3,4] Use of the PUP capability permits the SAMMY user to easily incorporate most of the experimental uncertainty into his or her analyses, thus providing a more realistic covariance matrix for the resulting set of resonance parameters.

Details for the IDC and PUP options will be given in this presentation, which will conclude with a discussion of other sources of uncertainty for which proper treatment is not yet understood or widely available. Among these are uncertainty in the theory itself (e.g., uncertainty due to a wrong spin assignment for a resonance) and the treatment of discrepant data.