VI.C.2. Explicit Data Covariance Matrices

Two types of options for off-diagonal data covariance matrices (DCM) are available within SAMMY. The first, which is labeled "explicit," is treated as a regular off-diagonal covariance matrix; see the description of Bayes' equations, Section IV. Use of the explicit data covariance matrix thus requires inversion of an $N \times N$ array, where N is the number of data points.

The second, "implicit" data covariance matrix (described in Section IV.A.1.a), makes use of the specific mathematical form for the covariance matrix,

$$V = v + g\, m\, g^t \quad , \tag{VI C2.1}$$

where v is the diagonal statistical portion, m is the covariance matrix for the data-reduction parameters, and g represents the partial derivatives of the theoretical values with respect to the data-reduction parameters. (See Section IV.D for more details.) With the implicit DCM, the components (v, g, and m) are provided to the code; V itself is not needed. The implicit DCM is treated by a more sophisticated mathematical process that does not require inversion of such a large matrix. See Section VI.C.3 for input details for the implicit DCM.

When either formulation could be used, the implicit is recommended because the implementation is far more efficient and often more accurate.

Table VI C2.1 shows the format for a Data CoVariance (DCV) file, to be included when each covariance matrix element is given explicitly. The name of this file must be specified in card set 3 of the INPut file (Tables VI A.1 and VI A1.2) in columns 31-40 of the line reading "`DATA COVARIANCE FILE is named ...`" Because the matrix is symmetric, only the lower triangular half of this matrix is given in the file; matrix elements are read across the columns, as illustrated here.

V11				
V21 ➔	V22			
V31 ➔	V32 ➔	V33		
V41 ➔	V42 ➔	V43 ➔	V44	
V51 ➔	V52 ➔	V53 ➔	V54 ➔	V55

When creating an explicit DCV file, it is important to provide as many significant digits as possible for each matrix element, in order to ensure reasonably accurate results and avoid numerical problems associated with singular matrices.

Occasionally it may be convenient to introduce a constant on- and off-diagonal data covariance in the neighborhood of a non-*s*-wave resonance, permitting effective decoupling of any underlying l = 0 state from the non-*s* waves. This is effective because an additive constant covariance is mathematically equivalent to a constant, coherent correction term for either the data or the theory. (Algebraic details are presented in Appendix A of the original SAMMY report [NL80].) This type of off-diagonal data covariance matrix can be generated automatically by SAMMY; details for input are given in Table VI A1.2 under the category "Experimental data – input control for covariance matrix" and in card set 1, columns 68 to 80, of Table VI B.2.

Another type of explicit off-diagonal data covariance matrix that can be automatically generated by SAMMY is of the form

$$V_{ij} = \bar{V}_{ij} + \left(a + bE_i\right)\left(a + bE_j\right) \quad , \qquad \text{(VI C2.2)}$$

where $\bar{V}_{ij}$ is provided by the user, E_i is the energy for data point i, and *a* and *b* are constants chosen by the user. This type of covariance is useful if there are energy-dependent coherent uncertainties in the data, for example, if a subtracted background is imperfectly known. Input for this option is given in card set 7 of Table VI A.2, and the "Input Control" statement "`DATA HAS OFF-DIAGONAL contribution ...`" of Table VI A1.2.

Table VI C2.1. Format of the data covariance file

This file contains the lower triangular half of the matrix, reading across the columns

Line	Column	Variable	Format	Meaning
1	1-10	VARDAT(1,1)	F10.1	Variance for data point 1
2	1-10	VARDAT(2,1)	F10.1	Covariance between data points 1 and 2
	11-20	VARDAT(2,2)	F10.1	Variance for data point 2
3	1-10	VARDAT(3,1)	F10.1	Covariance between data points 1 and 3
	11-20	VARDAT(3,2)	F10.1	Covariance between data points 2 and 3
	21-30	VARDAT(3,3)	F10.1	Variance for data point 3
4	1-10 ...	VARDAT(4,1) etc.	F10.1	
…				
Last	1-10 ...	VARDAT(Last,1) etc.	F10.1	

Note that the ordering of data points is **low** to **high** (independent of the ordering in the DATa file), and only those data points actually used in the calculation can be referenced in the DCV file. A maximum of eight matrix elements are to be included on one line; thus, "line number 11," for example, will actually be two lines, with eight numbers on the first and three on the second.