

### VI.C.3.b. User-supplied implicit data covariance matrix

After reducing experimental data from raw counts to a form resembling a cross section, the experimentalist has available all information needed to produce the covariance matrix for the reduced data. This covariance matrix would have the form given in Eq. (IVD.1):

$$V_{ij} = v_i \delta_{ij} + \sum_{kk'} g_{ik} m_{kk'} g_{jk'} \quad (\text{VI C3 b.1})$$

where  $g_{ik}$  is the partial derivative of the expression for data point  $i$  (in terms of the measured quantity and the data-reduction parameters) with respect to data-reduction parameter  $k$ . The covariance matrix for the data-reduction parameters is  $m$ . (For a concrete example of this, see the paper by Gunsing [FG98] detailing the derivation of the covariance matrix for data measured at the GELINA facility.)

Rather than generating the entire covariance matrix  $V$ , the SAMMY user can prepare a file containing the partial derivatives that SAMMY will then use for the Implicit Data Covariance Matrix. The SAMMY INPut file should contain the command “USER-SUPPLIED IMPLICIT data covariance matrix”, and the name of the file must be given directly after the name of the data file.

The format for the user-supplied implicit data covariance file is as shown in Table VI C3 b.1.

### Examples

For examples on the use of IDC, see test cases tr070, tr118, and tr140. Case tr118 contains equivalent examples of normalization and background included in the fitting (case a), implicit covariance matrix (cases c and i), user-supplied implicit data covariance matrix (cases g and h), and explicit data covariance matrix (case j).

**Table VI C3 b.1. Format for user-supplied IDC file**

Card set: Line	Variable	Meaning
1:1	Alpha	At least the first two characters (and the equal sign) of the phrase “NUMber of data-reduction parameters =”, followed by an integer number $K$ which indicates how many partial derivatives are to be read. Example: NU=7
1:2	(blank)	
2:1	Alpha	At least the first ten characters of the phrase “PARTIAL DERivatives” or “FREE-FORMAt partial derivatives”
2:2	X(i,1)	If “PARTIAL DERivatives”, then the $K$ partial derivatives for the first data point, eight values per line, continuing on the next lines if needed, in 8F10 format, or If “FREE-FORMAt partial derivatives”, then this line contains the energy, the statistical uncertainty on the first data point, and the $K$ partial derivatives for the first data point, in free format
2:3	X(i,2)	The $K$ partial derivatives for the second data point in 8F10 format, or Energy, statistical uncertainty, and partial derivatives in free format
etc.		
2: $N + 1$	X(i,N)	The $K$ partial derivatives for the $N$ th data point (where $N$ is the total number of data points in the SAMMY run), in 8F10 format. Energy, statistical uncertainty, and $K$ partial derivatives, in free format.
2: $N + 2$	(blank)	
3:1	Alpha	At least the first ten characters of the phrase “UNCERTAINTies on data-reduction parameters”. NOTE: This card set is optional and may be omitted if the uncertainties are multiplied into X, that is, if X(i,k) from card set 2 contains $X_k^i$ times the square root of $w_k$ rather than just $X_k^i$ itself.
3:2	X(i,1)	Uncertainties for the $K$ data-reduction parameters, continuing on the next lines if needed. Format is 8F10 or free-format as specified in card set 2, line 1.
3: 3	(blank)	
4:1	Alpha	At least the first ten characters of the phrase “CORRELATIONS for data-reduction parameters”. This card set is optional and may be omitted if values for the data-reduction parameters were independently determined (i.e., if parameters are uncorrelated).
4:2	C(1,2)	Correlation between parameter number 1 and parameter number 2. Format is F10 or free format, as specified in card set 2 line 1.
4:3	C(1,3), C(2,3)	Correlation between parameters 1 and 3, and between 2 and 3; format is 2F10 or free format.
etc.		
4: $K + 1$	C(i,K)	Correlation between parameters $i$ (for $i = 1$ to $K-1$ ) and $K$ , in 8F10 format or free format, continuing on additional lines if needed.
4: $K + 2$	(blank)	