QUALITY CHECKS INCLUDING EIGENVALUE TESTS ON THE LOW-FIDELITY COVARIANCE EVALUATION

D. W. Muir
Special Term Appointee
Argonne National Laboratory

INTRODUCTION

As part of the US effort to create a comprehensive, even if low-fidelity, covariance evaluation (Ref. 1), Argonne National Laboratory has the responsibility for performing an overall quality assurance of the file.

As part of this QA effort, we have performed an eigenvalue analysis of each of the symmetric LB=5 sub-subsections in the present version of the low-fidelity covariance evaluation.

For this study, we wrote a small, special-purpose checking code, starting from a collection of subroutines extracted from the GANDR system (Ref. 2).

SUMMARY OF NEGATIVE EIGENVALUES

We examined the covariance matrices associated with the LB=5 sub-subsections. We found **significant negative eigenvalues** in 44 of the 373 materials tested, around 12% of the files. By "significant", we mean negative eigenvalues that are much larger in absolute value than the small values that result from the rounding of covariances to 6 significant figures in formatted files.

MT	Eigenvalue	MATs with this Negative Eigenvalue in MT						
18	-3.897E-02	8931	9025	9028	9031	9034	9043	9046
		9134	9219	9340	9343	9349	9352	9428
		9431	9449	9452	9458	9552	9553	9628
		9649	9652	9655	9752	9755	9852	9855
		9858	9861	9867	9914	9915	9936	
18	-9.743E-03	9131	9137	9234	9240	9243	9246	9546
		9643	9646					
102	-6.336E-03	528						

The frequent repetitions of just two negative eigenvalues, -3.897E-02 and -9.743E-03, in the list above is the result of including the very same relative covariance matrix in many fissionable materials in the Low-fidelity data set. The 34 evaluations listed above as having an eigenvalue of -3.897E-02 all have the same 12-energy-bin covariance matrix for the fission reaction (MT=18, MT1=18). This matrix is shown below.

Relative Covariance for All MATs with Eigenvalue -3.897E-02

.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
.000	.090	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
.000	.000	.090	.072	.072	.072	.000	.000	.000	.000	.000	.000
.000	.000	.072	.090	.072	.072	.000	.000	.000	.000	.000	.000
.000	.000	.072	.072	.090	.072	.000	.000	.000	.000	.000	.000
.000	.000	.072	.072	.072	.090	.072	.072	.072	.000	.000	.000
.000	.000	.000	.000	.000	.072	.090	.072	.072	.000	.000	.000
.000	.000	.000	.000	.000	.072	.072	.090	.072	.000	.000	.000
.000	.000	.000	.000	.000	.072	.072	.072	.090	.072	.072	.072
.000	.000	.000	.000	.000	.000	.000	.000	.072	.090	.072	.072
.000	.000	.000	.000	.000	.000	.000	.000	.072	.072	.090	.072
.000	.000	.000	.000	.000	.000	.000	.000	.072	.072	.072	.090

ANALYSIS

This covariance matrix is mainly block diagonal, but with three **overlapping** blocks. This is possible if there are 3 independent sources of error, and
(1) one source induces a fully correlated covariance of size 0.072 in bins 3-6,
(2) a second induces a fully correlated covariance of size 0.072 in bins 6-9,
(3) a third induces a fully correlated covariance of size 0.072 in bins 9-12.
One can begin by adding these three partial covariance matrices together.

It appears that there is an additional, fully uncorrelated source of error that
(1) increases the variances in all energy bins from 3 to 12,
(2) has a constant magnitude of 0.018.
This diagonal matrix can be added to the previous matrix.

These steps reproduce the data values shown in color above, except for groups 6 and 9, where the diagonal elements (variances) have the **wrong value**,
$\mathrm{cov}(a_6,a_6) = \mathrm{cov}(a_9,a_9) =$ `0.072 + 0.072 + 0.018 = 0.162`
To correct for this, we have to add, along the diagonal, additional variances that are zero everywhere except in the (6,6) and (9,9) positions. To get the desired matrix shape, they would have to have the (impossible) values of `-0.072`!

The best way to detect occurrences of mathematically impossible covariance matrices like this is to calculate the **eigenvalues** of covariance matrices of interest. An *n x n* covariance matrix has *n* eigenvalues.

Each eigenvalue is represents the variance of a set of *n* effectively independent linear combinations of the parameters. The specific linear combination associated with a given eigenvalue is defined by the **eigenvector** associated with that eigenvalue.

To make this clearer, consider a simple 3-parameter problem with the following covariance matrix, obviously related to the fission cross section covariances discussed above.

```
                0.090    0.072    0.000
D(a) =    [     0.072    0.090    0.072 ]
                0.000    0.072    0.090
```

Note that parameter 2 is part of the 1-2 "correlated block" and part of the 2-3 "correlated block." The eigenvalues of this matrix are `-1.1823E-02`, `9.0000E-02`, and `1.9182E-01`. The eigenvector associated with the negative eigenvalue is

```
V = [ 5.0000E-01 -7.0711E-01  5.0000E-01 ]
```

Consider that there exists an integral quantity z

$$z = \mathbf{S}\,\mathbf{a}$$

where the sensitivity matrix **S** contains the following values:

$$\mathbf{S} = \mathbf{V} = \begin{bmatrix} 0.5 & -0.5^{1/2} & 0.5 \end{bmatrix}$$

By the usual "sandwich rule" of error propagation, the variance of z is

$$D(z) = \mathbf{S}\, D(\mathbf{a})\, \mathbf{S}^T = \sum_{i,j=1,k} d_{ij}\, S_i\, S_j$$

$$= \begin{matrix} 0.090*0.5*0.5 & -0.072*0.5*0.5^{1/2} & +0.0 \\ -0.072*0.5*0.5^{1/2} & +0.090*0.5 & -0.072*0.5*0.5^{1/2} \\ +0.0 & -0.072*0.5*0.5^{1/2} & +0.090*0.5*0.5 \end{matrix}$$

$$= 0.090 - 0.072*2^{1/2}$$

$$D(z) = -1.1823E{-}02$$

Thus for the particular function z of the parameters **a**, the specified covariance matrix yields a negative variance (and hence imaginary standard deviation), which is obviously non-physical. Note that the numerical value of the variance of z is exactly equal to the troublesome negative eigenvalue.

ISSUES NOT RELATED TO EIGENVALUES

In the course of the processing of the low-fidelity covariance files, a few clerical errors were found, and these points are summarized below.

A. ^{6}Li (MAT=325), MT=2

In ^{6}Li (MAT325), MT=2, the NI-type sub-subsection with LB=5 has the value of 0 as the lowest energy in the grid, instead of the required 1.e-5 eV.

B. ^{nat}C (MAT=600), (MT,MT1)= (4,4)
^{14}N (MAT=725), (MT,MT1)= (4,4)
^{16}O (MAT=825), (MT,MT1)= (4,4)

Each of the listed covariance subsections contain an NC-type sub-subsection indicating that MT=4 was evaluated as a difference between the total cross section and the nonelastic over the energy range from 1.e-5 eV to 20 MeV. At the same time, it an NI-type sub-subsection covering the energy range from 1.e-5 to 150 MeV. According to Para. 33.3.3.3 in the manual, the "F-values" in the NI-type sub-subsection must be zero in any energy region covered by both NI-type and NC-type sub-subsections. In fact, the evaluator has set to <u>all</u> the covariances in the NI-type sub-subsection equal to zero. A better approach would be to remove it.

C. ^{19}F (MAT=925), MT= 4, 16, 22 and 28

The evaluation for ^{19}F raises a number of interesting issues. For one thing, it includes a sub-subsection with LB=8 in each of the self-reaction subsections. In the current manual, the inclusion of LB=8 is encouraged as a general practice. However, LB=8 is easy to mis-use, and there is little apparent practical need for it. For these reasons, **I recommend against the widespread use of LB=8**.

The evaluation includes subsections for the reaction pairs (4,16), (4,22), (4,28), (16,22), (16,28) and (22,28). In each of these subsections, covariances are stored in an NI-type sub-subsection with LB=5, with the symmetry flag LS set to 0 (asymmetric matrix). This combination is not recommended for general use, because only a single energy grid is provided, with NE energies. A square array of dimension (NE-1)*(NE-1) contains the covariances, and the identical energy grid is used for both MT and MT1. For example, in the ^{19}F subsection (4,4), the energy grid includes 12 energies ranging from 115.84 keV to 20 MeV. In the (4,16) subsection, on the other hand, the same reaction MT = 4 is represented on a grid that includes only 6 energies ranging from 10.985 MeV to 20 MeV, the same as MT = 16. **For all between-reaction covariances, I recommend against using NI-type sub-subsections with LB=5 (use LB=6 instead)**. This permits entry of a rectangular matrix, so each of the reactions can be represented on an appropriate energy grid.

GENERAL COMMENT REGARDING COMBINING LB=1 WITH LB=5

Many of the evaluations in the low-fidelity file include, in the self-reaction subsections, both an NI-type sub-subsection with LB=1 and one with LB=5. This is not illegal, but it seems a little illogical.

If an evaluation includes a sub-subsection that treats a portion of the total covariance with the general matrix capability of LB=5, what is the advantage of adding a separate sub-subsection employing the simplified LB=1 block-diagonal format? Why not just add the two components together to create a new LB=5 matrix?

This would make the file more human-readable. For example, when only the LB=5 format is employed, the complete energy grid used in the covariance evaluation is stored a single vector array.

As a general practice, I recommend against including both LB=1 and LB=5 sub-subsections in the same subsection.

CONCLUSION

As part of the US effort to create a comprehensive, but low-fidelity, covariance evaluation, Argonne National Laboratory has the responsibility for performing an overall quality assurance of the file.

As part of this QA effort, we have performed an eigenvalue analysis of each of the symmetric LB=5 sub-subsections in the present version of the low-fidelity covariance evaluation. This effort has revealed the existence of 44 evaluations with significant negative eigenvalues. The reason is traced to the inclusion of overlapping regions of high correlation in many of the evaluations. These matrices should be modified to avoid this problem.

We also list some other areas where the quality of the files can be improved.

REFERENCES

1. R.C. Little et al., "Low-fidelity Covariance Project," Workshop on Neutron Cross Section Covariances, Port Jefferson, NY, June 24-27, 2008.
2. D.W. Muir, "Global Assessment of Nuclear Data Requirements: the GANDR Project," www-nds.iaea.org/gandr/codes.html.