Covariance Testing on U-235, U-238, and Pu-239 in ENDF/B VIII.1 Beta1

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Outline

- Basics of Covariance Testing
- Covariance Testing Procedure
- Results for U-235, U-238, and Pu-239
- Summary

Covariance Testing in General

- Covariance Matrices should be non-negative definite symmetric
  - i.e., **no negative eigenvalues**
    - Check by eigenvalue decomposition
    - Or, Check by matrix square root – are the output elements real or complex?
    - Or, Check by inspecting correlation matrices – are they valid?
- **Two Covariance Constraints that need to be satisfied**
  - In MF 33 – cross sections
    - *Because the Total cross section = sum of partial cross sections*
    - Absolute Covariance of Total = sum of the abs. covariances of the partial cross sections
  - In MF 35 – fission chi – beware of numerical precision issues
    - *Because the Sum of multigroup chi's = 1.0*
    - Absolute Covariance matrix should have zero-sum and zero-column conditions
  - These 2 constraints are related – see my recent ND paper.

Covariance Testing of U-235, U-238, Pu-239

- **Use NJOY to create 30g cross sections and covariances**
  - Follow-up testing could investigate the covariance properties on the native energy bin structure in the evaluation file
- **Use the ASCII interface file output from ERRORR** – since it has more numerical precision than the printed output or other formats (e.g., BOXER)
- **Read the ERRORR interface files with simple FORTRAN programs**
  - 6F11.0 format in FORTRAN will read the old-fashioned ENDF-6 formats
- **Use Excel** for visualization, group sums, and data transfers
- **Use MATLAB for numerical operations** like eigenvalue decomposition, matrix square roots, covariance and correlation conversions, etc
- (**O16** results presented in Nathan Gibson's paper.)

U-235 Results

- MF 31 – nu
  - **Some small, but annoying negative eigenvalues were seen**
    - Believed to be a result of inconsistent merging of the covar. data
  - Illegal values were also seen in the associated correlation matrices
- MF 33 – cross sections
  - Cross section balance and covariance balance were ok
    - Covariance balance was keyed to MT 1
  - Combined big covariance matrix had only very small neg. eigenvalues
- MF 34 – mubar
  - Values of mubar within -1.0 to 1.0, also std.dev < 1.0
  - No negative eigenvalues
- MF 35 – fission chi (tested at efmean = 2.5e6 eV)
  - Multigroup-chi's summed to 1.0
  - **Relative Covariance matrix had negative eigenvalues, but the absolute covariance matrix did not – indicating problems with small values and roundoff**

U-238 Results

- MF 31 – nu
  - No negative eigenvalues were seen
- MF 33 – cross sections
  - Cross section balance and covariance balance were ok
    - Covariance balance was keyed to MT 1
  - Combined big covariance matrix had only very small neg. eigenvalues
- MF 34 – mubar
  - Values of mubar within -1.0 to 1.0, also std.dev < 1.0
  - No negative eigenvalues
- MF 35 – fission chi (tested at efmean = 2.5e6 eV)
  - Multigroup-chi's summed to 1.0
  - **Relative Covariance matrix had negative eigenvalues, but the absolute covariance matrix was not quite symmetric – *drowning* in round-off errors.**

Pu-239 Results

- MF 31 – nu
  - **Some small, but annoying negative eigenvalues were seen (cf U-235)**
  - Illegal values were also seen in the associated correlation matrices
  - Identical covariances for MT 452 (total) and MT 456 (prompt)
  - **Empty gap in covariance data between 2.50e3 and 4.00e3 eV**
- MF 33 – cross sections
  - Cross section balance was ok
    - **But covariance constraint was not satisfied at E < 3.5e3 eV**
    - Above 3.5e3 eV, constraint was keyed to MT 2
  - Combined big covariance matrix had only very small neg. eigenvalues
- MF 34 – mubar
  - *No covariance data was given in Beta 1 –> see Beta 1.1*
- MF 35 – fission chi (tested at efmean = 2.5e6 eV)
  - Multigroup-chi's summed to 1.0
  - **Relative Covariance matrix had negative eigenvalues, but the absolute covariance matrix did not – indicating problems with small values and round-off errors.**

SUMMARY

- Some work remains to be done with the covariance data of O-16, U-235, U-238, and Pu-239 …
- **But we are making progress!**

- For how to meet the MF 33 covariance constraint:
  - See the ENDF-6 Manual

    A. Trkov, M. Herman, and D.A. Brown, "The ENDF-6 Formats Manual", BNL-90365-2009 Rev. 2, or CSEWG ENDF-102, Brookhaven National Laboratory, (2012).
  - See my ND 2022 paper

    Includes procedural and normalization instructions