Fission Spectrum Covariance in Uncertainty Analyses

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Outline

- Background
- Covariance matrix in File 35 of ENDF
  - Normalization scheme
- Sensitivity coefficient calculation methods
  - Unconstrained sensitivity coefficients
  - Constrained sensitivity coefficients
- Equivalence of unconstrained and constrained sensitivity coefficients
  - Response parameter variation
  - Response parameter uncertainty
- Impacts of numerical precision of covariance matrix
- Conclusions

Background

- The impact of the fission spectrum uncertainty on the multiplication factor uncertainty was previously investigated for the sodium-cooled ABTR and the KRITZ thermal benchmark experiment
  - G. Aliberti, I. Kodeli, G. Palmiotti, M. Salvatores, "Fission Spectrum Related Uncertainties," NEMEA-4 Conference, Prague, October 16-18, 2007
- Significantly high uncertainties (~4%) were reported
  - Such high uncertainties exceed the typical uncertainties associated with the cross sections, and would impose important restrictions on the reactor design
- Inconsistencies in the sensitivity calculation methods and/or in the covariance matrix evaluation and processing were suggested as a possible explanation for the high uncertainties
- Consistent usage of fission spectrum covariance matrices and sensitivity coefficients for response parameter uncertainty estimation was presented
  - W. S. Yang, G. Aliberti, R. D. McKnight, and I. Kodeli, "Fission Spectrum Covariance Matrix and Sensitivity Coefficients for Response Parameter Uncertainty Estimation," Workshop on Neutron Cross Section Covariances, Port Jefferson, New York, June 24-27, 2008

Properties of Covariance Matrix in File 35

- **Fission spectrum**

$$\sum_{i=1}^{n} \chi_i = 1$$

$$\mathbf{u}^T \boldsymbol{\chi} = \boldsymbol{\chi}^T \mathbf{u} = 1, \quad \mathbf{u} = (1, 1, \cdots, 1)^T$$

- **Covariance matrix**

$$\sigma_{ij} = (\mathbf{V}_\chi)_{ij} = < (\chi_i - \bar{\chi}_i)(\chi_j - \bar{\chi}_j) >$$

  - Symmetric
  - Positive definite
  - Zero column or row sum

$$\sum_{i=1}^{n} \sigma_{ij} = 0 \ \text{ or } \ \sum_{j=1}^{n} \sigma_{ij} = 0$$

Renormalization of Covariance Matrix in File 35

- **Normalization scheme specified in File 35 of ENDF**

$$\tilde{\sigma}_{ij} = \sigma_{ij} - \chi_i \sum_k \sigma_{kj} - \chi_j \sum_k \sigma_{ki} + \chi_i \chi_j \sum_k \sum_l \sigma_{kl}$$

- **Congruent transformation**

$$\tilde{\sigma}_{ij} = \sum_k \sum_l (\delta_{ki} - \chi_i) \sigma_{kl} (\delta_{lj} - \chi_j)$$

$$\tilde{\mathbf{V}}_\chi = \mathbf{P}^T \mathbf{V}_\chi \mathbf{P}$$

$$\mathbf{P} = \mathbf{I} - \mathbf{u}\boldsymbol{\chi}^T$$

- $\mathbf{P}$ is an oblique projection operator
  - *Range:* $L = \{\mathbf{x} \in \mathbb{R}^n \mid \boldsymbol{\chi}^T \mathbf{x} = 0\}$
  - *Null space:* $U = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x} = \alpha \mathbf{u}, \alpha \in \mathbb{R}\}$

$$\mathbf{P}^2 = \mathbf{P}$$

Sensitivity Coefficients

- **Unconstrained sensitivity coefficients**
  - Gradient of a response at the point of nominal fission spectrum

$$\mathbf{s}_{\chi} = \nabla R(\boldsymbol{\chi}) = \left(\frac{\partial R}{\partial \chi_1}, \frac{\partial R}{\partial \chi_2}, \cdots, \frac{\partial R}{\partial \chi_n} \right)^T$$

- **Constrained sensitivity coefficients (SAGEP of JAEA)**
  - Perturbed fission spectrum is constrained to satisfy the fission spectrum normalization condition
  - Equivalent to the projection of the gradient on the surface representing the fission spectrum normalization condition

$$\tilde{\mathbf{s}}_{\chi} = \mathbf{P}\mathbf{s}_{\chi}$$

Equivalence of Constrained and Unconstrained Sensitivity Coefficients for Response Parameter Uncertainty Evaluation

- **Response variation computed with constrained sensitivity coefficients**

$$\delta R = \tilde{\mathbf{s}}_\chi^T \delta\boldsymbol{\chi} = (\mathbf{P}\mathbf{s}_\chi)^T \delta\boldsymbol{\chi} = \mathbf{s}_\chi^T \mathbf{P}^T \delta\boldsymbol{\chi} = \mathbf{s}_\chi^T \delta\boldsymbol{\chi}$$

- **Response uncertainty computed with constrained sensitivity coefficients**

$$\sigma_R^2 = \tilde{\mathbf{s}}_\chi^T \mathbf{V}_\chi \tilde{\mathbf{s}}_\chi = (\mathbf{P}\mathbf{s}_\chi)^T \mathbf{V}_\chi (\mathbf{P}\mathbf{s}_\chi) = \mathbf{s}_\chi^T \mathbf{P}^T \mathbf{V}_\chi \mathbf{P}\mathbf{s}_\chi = \mathbf{s}_\chi^T \tilde{\mathbf{V}}_\chi \mathbf{s}_\chi$$

$$\tilde{\mathbf{V}}_\chi = \mathbf{P}^T \mathbf{V}_\chi \mathbf{P}$$

  - Equivalent to normalizing the covariance matrix to satisfy the zero-sum constraint

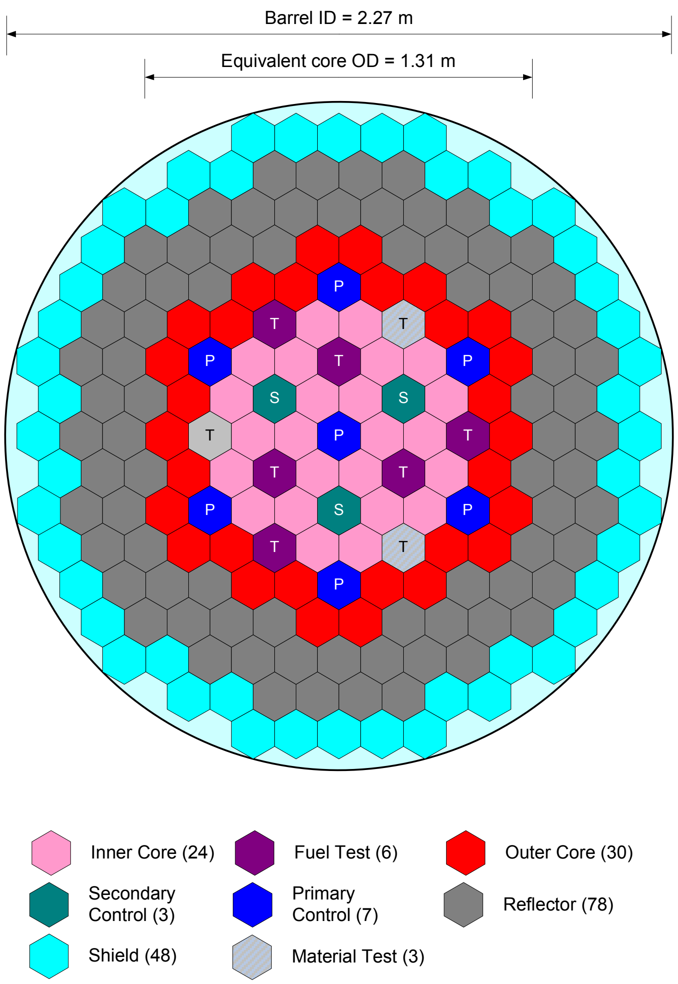
$$\mathbf{P}^T \tilde{\mathbf{V}}_\chi \mathbf{P} = (\mathbf{P}^T)^2 \mathbf{V}_\chi \mathbf{P}^2 = \mathbf{P}^T \mathbf{V}_\chi \mathbf{P} = \tilde{\mathbf{V}}_\chi$$

  - When a covariance matrix satisfies the zero sum constraint as required, constrained and unconstrained sensitivity coefficients yield the same uncertainty

Numerical Example of ABTR

- Sensitivity coefficients of multiplication factor w.r.t. Pu-239 fission spectrum

Energy group	Upper boundary (eV)	Fission spectrum	Sensitivity coefficients	
			unconstrained	constrained
1	1.96E+07	0.03089	0.03236	0.00785
2	6.07E+06	0.33969	0.29489	0.02534
3	2.23E+06	0.23100	0.18798	0.00468
4	1.35E+06	0.28041	0.20084	-0.02167
5	4.98E+05	0.08958	0.06010	-0.01098
6	1.83E+05	0.02192	0.01368	-0.00371
7	6.74E+04	0.00505	0.00284	-0.00117
8	2.48E+04	0.00113	0.00061	-0.00029
9	9.12E+03	0.00029	0.00017	-0.00006
10	2.03E+03	0.00003	0.00002	0.00000
11	4.54E+02	0.00000	0.00000	0.00000
12	2.26E+01	0.00000	0.00000	0.00000
13	4.00E+00	0.00000	0.00000	0.00000
14	5.40E-01	0.00000	0.00000	0.00000
15	1.00E-01	0.00000	0.00000	0.00000
sum		1.00001	0.79350	0.00000



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Un-normalized Covariance Matrix

Relative STD	Correlation															
	Gr.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0.09692	1	1.000	0.846	-0.326	-0.923	-0.671	-0.608	-0.590	-0.587	-0.587	-0.587	-0.590	-0.593	-0.593	-0.593	-0.593
0.03475	2	0.846	1.000	0.227	-0.986	-0.963	-0.937	-0.929	-0.928	-0.928	-0.928	-0.930	-0.931	-0.931	-0.931	-0.931
0.01026	3	-0.326	0.227	1.000	-0.062	-0.482	-0.552	-0.571	-0.574	-0.574	-0.574	-0.571	-0.568	-0.568	-0.568	-0.568
0.02707	4	-0.923	-0.986	-0.062	1.000	0.905	0.867	0.855	0.853	0.853	0.853	0.855	0.857	0.857	0.857	0.857
0.05358	5	-0.671	-0.963	-0.482	0.905	1.000	0.997	0.995	0.994	0.994	0.994	0.995	0.995	0.995	0.995	0.995
0.06344	6	-0.608	-0.937	-0.552	0.867	0.997	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06726	7	-0.590	-0.929	-0.571	0.855	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06436	8	-0.587	-0.928	-0.574	0.853	0.994	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06732	9	-0.587	-0.928	-0.574	0.853	0.994	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06420	10	-0.587	-0.928	-0.574	0.853	0.994	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06437	11	-0.590	-0.930	-0.571	0.855	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06282	12	-0.593	-0.931	-0.568	0.857	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06321	13	-0.593	-0.931	-0.568	0.857	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06367	14	-0.593	-0.931	-0.568	0.857	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06097	15	-0.593	-0.931	-0.568	0.857	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Normalized Covariance Matrix

Relative STD	Correlation															
	Gr.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0.09604	1	1.000	0.843	-0.426	-0.918	-0.670	-0.607	-0.589	-0.586	-0.586	-0.586	-0.589	-0.592	-0.592	-0.592	-0.593
0.03369	2	0.843	1.000	0.126	-0.988	-0.964	-0.939	-0.931	-0.930	-0.929	-0.930	-0.931	-0.932	-0.932	-0.932	-0.933
0.01004	3	-0.426	0.126	1.000	0.033	-0.386	-0.460	-0.480	-0.482	-0.482	-0.482	-0.478	-0.475	-0.475	-0.476	-0.475
0.02811	4	-0.918	-0.988	0.033	1.000	0.910	0.873	0.861	0.860	0.860	0.860	0.862	0.864	0.864	0.864	0.864
0.05461	5	-0.670	-0.964	-0.386	0.910	1.000	0.997	0.995	0.994	0.994	0.994	0.995	0.995	0.995	0.995	0.995
0.06444	6	-0.607	-0.939	-0.460	0.873	0.997	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06825	7	-0.589	-0.931	-0.480	0.861	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06536	8	-0.586	-0.930	-0.482	0.860	0.994	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06832	9	-0.586	-0.929	-0.482	0.860	0.994	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06519	10	-0.586	-0.930	-0.482	0.860	0.994	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06538	11	-0.589	-0.931	-0.478	0.862	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06383	12	-0.592	-0.932	-0.475	0.864	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06421	13	-0.592	-0.932	-0.475	0.864	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06467	14	-0.592	-0.932	-0.476	0.864	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.06198	15	-0.593	-0.933	-0.475	0.864	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Covariance Matrix Change by Normalization

Relative STD	Correlation															
	Gr.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
-0.00088	1	0.000	-0.003	-0.100	0.005	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.000
-0.00106	2	-0.003	0.000	-0.101	-0.002	-0.001	-0.002	-0.002	-0.002	-0.001	-0.002	-0.001	-0.001	-0.001	-0.001	-0.002
-0.00022	3	-0.100	-0.101	0.000	0.095	0.096	0.092	0.091	0.092	0.092	0.092	0.093	0.093	0.093	0.092	0.093
0.00104	4	0.005	-0.002	0.095	0.000	0.005	0.006	0.006	0.007	0.007	0.007	0.007	0.007	0.007	0.007	0.007
0.00103	5	0.001	-0.001	0.096	0.005	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00100	6	0.001	-0.002	0.092	0.006	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00099	7	0.001	-0.002	0.091	0.006	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00100	8	0.001	-0.002	0.092	0.007	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00100	9	0.001	-0.001	0.092	0.007	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00100	10	0.001	-0.002	0.092	0.007	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00100	11	0.001	-0.001	0.093	0.007	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00100	12	0.001	-0.001	0.093	0.007	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00100	13	0.001	-0.001	0.093	0.007	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00100	14	0.001	-0.001	0.092	0.007	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00100	15	0.000	-0.002	0.093	0.007	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Effects of Numerical Precision of Covariance Matrix

- There was a concern about the numerical precision of covariance matrix
  - Need to change ENDF format from single precision to double precision?
- In order to examine the numerical precision effects of the covariance matrix, the eigensystem was examined by varying the number of significant digits

Covariance matrix	Un-normalized		Normalized		
	3 digits	round-off	5 digits	4 digits	3 digits
Eigenvalue	2.25367E-04	7.80063E-08	2.22173E-04	2.22172E-04	2.22202E-04
	1.12404E-05	3.35946E-08	1.11465E-05	1.11465E-05	1.11455E-05
	1.77653E-08	1.16609E-08	-1.42449E-08	-1.44125E-08	2.03517E-08
	-1.44862E-08	4.70302E-09	1.12976E-08	1.12228E-08	-1.31572E-08
	4.64998E-09	3.53774E-09	-2.25217E-09	-2.36182E-09	4.79453E-09
	-3.73921E-09	1.08106E-09	-1.01306E-11	-1.00632E-10	-1.83992E-09
	-4.00757E-11	-1.34503E-13	4.32903E-12	-9.77645E-12	1.42987E-11
Max. row sum	1.24985E-05	8.21081E-08	6.30385E-11	2.46947-10	4.46745E-08

- **Eigenvalues in descending order in absolute value**

Multiplication Factor Uncertainties

- With the normalized covariance matrix, both the unconstrained and constrained sensitivity coefficients yield the same uncertainties
  - Duplicated use of the normalization condition in sensitivity calculation and covariance matrix generation does not change the result
- Imposition of the fission spectrum normalization condition on sensitivity coefficient calculation is equivalent to renormalizing the covariance matrix of fission spectrum to satisfy the zero-sum constraints
- Numerical precision of covariance matrix appears to be of minor importance, when it is normalized to satisfy the zero-sum constraints

Sensitivity Coefficients	Covariance Matrix			
	Un-normalized	Normalized		
	3 digits	5 digits	4 digits	3 digits
Unconstrained	3.84012E-03	3.00003E-03	2.99997E-03	3.00499E-03
Constrained	3.00003E-03	3.00003E-03	3.00003E-03	3.00006E-03

Conclusions

- The method to renormalize the covariance matrix to satisfy the zero-sum constraint is a congruent transformation of the covariance matrix using the oblique projection operator that maps the normalized fission spectrum space onto itself
  - When the covariance matrix is already normalized, this transformation does not change the covariance matrix
- Imposition of the fission spectrum normalization condition on sensitivity coefficient calculation is equivalent to renormalizing the covariance matrix to satisfy the zero-sum constraints
- Both unconstrained and constrained sensitivity coefficients yield the same response uncertainty when a normalized covariance matrix is used
  - If an un-normalized covariance matrix is used, the constrained sensitivity coefficients yield the correct response uncertainty
- Numerical precision of covariance matrix appears to be of minor importance, when it is normalized to satisfy the zero-sum constraints