



SAMMY Workshop

Part 4.3

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Part 4.3, Fitting Procedure

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OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

3. Fitting procedure

(Bayes' Method)

Fitting procedure

- **SAMMY uses Bayes' Equations rather than Least Squares**
 - See Section IV in SAMMY Users' Manual (R7)
- **Bayes' Equations are sometimes called “Generalized Least Squares”**
- **Alternatively, Least Squares can be viewed as a special case of Bayes' Equations**

Basis for Bayes' Equations

- Bayes' equations are based on Bayes' Theorem:

$$p(P|DB) \propto p(P|B) p(D|PB)$$

where

$p(a|b)$ = probability that a is true, given that b is true

P = parameters whose values are to be determined

D = experimental data to be analyzed

B = all other relevant information

~~probability density functions (pdfs)~~ are defined as

$p(P|B)$ = prior pdf for the parameters

$p(P|DB)$ = posterior pdf for the parameters

$p(D|PB)$ = pdf for observing data D , given that P are correct

= maximum likelihood function

Bayes' Equations, cont.

$$\boxed{\text{Bayes' Theorem}} + \boxed{\text{three assumptions}} + \boxed{\text{algebra}} = \boxed{\text{Bayes' Equations}}$$

- **Assumptions**

Not one of these assumptions is true ...

- Prior joint probability density function $p(P|B)$ is a joint normal.
- Likelihood function $p(D|PB)$ is a joint normal.
- True value is a **linear function** of the parameters.

The theoretical cross section is *not* a linear function of the R-matrix parameters!

- **Derivation**

- Given in the users' guide
- Results only will be shown here

... but all are close enough to "true" to be useful.

Bayes' Equations (explicitly)

$$\begin{aligned} P' &= P + M' \boxed{Y} & M' &= (M^{-1} + \boxed{W})^{-1} \\ \boxed{Y} &= G^t V^{-1} (D - T) & \boxed{W} &= G^t V^{-1} G \end{aligned}$$

Goal of analysis:
find P' and M'

Notation: (primes indicate updated values)

P = parameters

M = covariance matrix for parameters

D = experimental data

T = theoretical calculation

G = partial derivatives (sensitivity matrix)

V = covariance matrix for experimental data

Compare to least squares -

Bayes' equations	Least Squares
$P' = P + M' Y$ $Y = G^t V^{-1} (D - T)$	$M' = (M^{-1} + W)^{-1}$ $W = G^t V^{-1} G$ $M' = W^{-1}$
M = initial covariance matrix for parameters	M = infinite and diagonal, “no prior knowledge”
Remembers earlier results	Forgets
Use results of one analysis as input to another	Cannot
Results from sequential analyses are “identical” to those obtained from simultaneous analysis (subject to linearity restrictions)	Not
OK to vary irrelevant parameters; values and uncertainties will change only slightly	Fitting procedure wastes time trying to find “good values” for irrelevant parameters

Review: Covariance vs Correlation

$$C_{ij} = \langle \delta P_i \delta P_j \rangle = \Delta P_i c_{ij} \Delta P_j$$

where

C_{ij} is the covariance matrix element between parameters P_i and P_j

ΔP_i is uncertainty on P_i

c_{ij} is the correlation coefficient between P_i and P_j

- Value of correlation coefficient is always between -1 and +1 :

$$-1 \leq c_{ij} \leq +1$$

Also always $|C_{ij}| \leq \Delta P_i \Delta P_j$

Why bother with covariances?

- Integral Quantities are needed for reactor applications

$$\int_{E_{min}}^{E_{max}} \sigma(E) \varphi(E) dE$$

where

- $\varphi(E)$ can be flux or any other function
 - $\sigma(E)$ is cross section, calculated from resonance parameters
 - E_{min} to E_{max} can be a large energy range (perhaps 0 to infinity)
-
- Uncertainties on these integral quantities are also needed.
 - Calculation of uncertainties on integral quantities requires knowledge of the uncertainties on the quantities within the integrand – and also knowledge of the covariances relating those uncertainties.

Example: Why covariances are important

Simple example: a straight line

- Suppose a “data fitting program” has found values, uncertainties, and correlation for a and b . That is,

$$\langle a \rangle = A$$

$$\langle (\delta a)^2 \rangle = \Delta^2 A$$

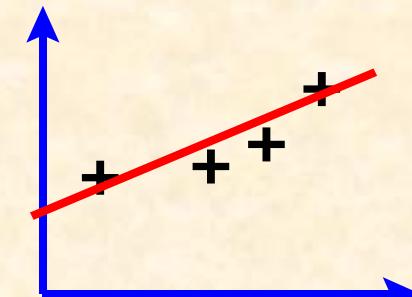
$$\langle b \rangle = B$$

$$\langle (\delta b)^2 \rangle = \Delta^2 B$$

$$\langle \delta a \delta b \rangle = \Delta A \Delta B c$$

(c is the correlation coefficient between A and B)

$$\sigma(E) = a E + b$$



Example: straight line, continued

- Then suppose the integral quantity of interest is

$$y = \frac{1}{E_{max} - E_{min}} \int_{E_{min}}^{E_{max}} \sigma(E) dE = \frac{1}{E_{max} - E_{min}} \int_{E_{min}}^{E_{max}} (aE + b) dE$$

$$= \frac{1}{E_{max} - E_{min}} \left(a \frac{E_{max}^2 - E_{min}^2}{2} + b(E_{max} - E_{min}) \right)$$

$$= a\boxed{\varepsilon} + b$$

where $\boxed{\varepsilon}$ is the midpoint of the range, $\varepsilon = (E_{max} + E_{min})/2$

Example: straight line, continued

- Expected value of y is $Y = (A\varepsilon + B)$. What is uncertainty on Y ?
- Uncertainties are “propagated” by taking small increments, squaring, and taking expectation values.

$$\delta y = \delta a \varepsilon + \delta b$$

$$\begin{aligned}\langle (\delta y)^2 \rangle &= \langle (\delta a \varepsilon + \delta b)^2 \rangle \\ &= \langle (\delta a)^2 \rangle \varepsilon^2 + 2\langle \delta a \delta b \rangle \varepsilon + \langle (\delta b)^2 \rangle\end{aligned}$$

- Rewriting this gives

$$\Delta^2 Y = \varepsilon^2 \Delta^2 A + 2\varepsilon c \Delta A \Delta B + \Delta^2 B$$

where range on c is -1 to +1. Usual approximation: $c = 0$

Example: straight line, continued

- TRY SOME NUMBERS...

$$A = 100 \pm 10, B = 40 \pm 5, E_{min} = 0.5, E_{max} = 1.5 \text{ so } \varepsilon = 1.0$$

$$Y = (1)(100) + (40) = 140$$

$$\Delta^2 Y = (1)^2 (10)^2 + (5)^2 + 2(1)c(10)(5) = 125 + 100c$$

$c = 0$ implies $\Delta Y = 11.18$

$c = 1$ implies $\Delta Y = 15.00$

$c = -1$ implies $\Delta Y = 5.00$

Proper use of covariance information can make a BIG difference in the final results!

Therefore $Y \pm \Delta Y = 140.00 \pm 5.00$ if $c = -1$

$= 140.00 \pm 11.18$ if $c = 0$

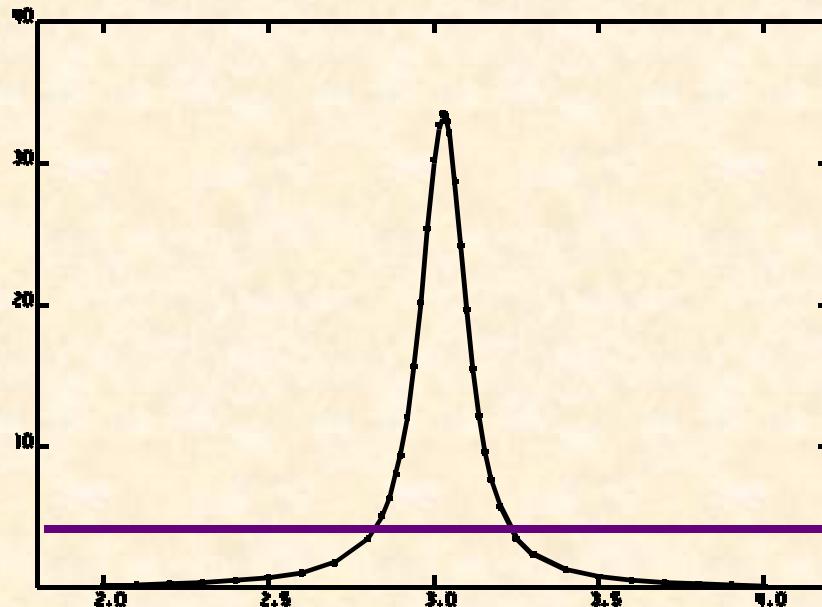
$= 140.00 \pm 15.00$ if $c = 1$

Unc $\sim 4\%$

Unc $\sim 8\%$

Unc $\sim 11\%$

More realistic example

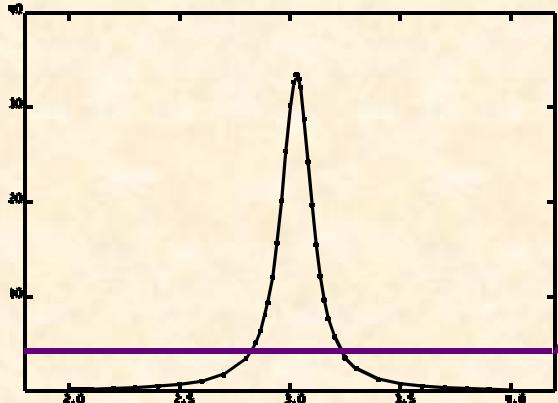


Wanted: to find the average value of this cross section

Uranium-like sample, fission cross section, one resonance

**Crosses = fission “data” for this example
Solid Curve = SAMMY fit to the data**

More realistic example, continued



**Group Cross Section
(averaged from 2 to 4 eV):**
With covariances:
 4.028 ± 0.026 barns (0.6%)
Without covariances:
 4.028 ± 1.061 barns (26%)

Proper use of covariance information can make a BIG difference in the final results!

Fitted values for resonance parameters –

	Fitted values (eV)	Correlation Matrix ×
100		
E_0	3.03038 \pm 0.00006	100
Γ_γ	0.051323 \pm 0.01952	0 100
Γ_n	0.0000218 \pm 0.0000044	0 100 100
Γ_{f1}	-0.036825 \pm 0.01720	0 -31 -31 100
Γ_{f2}	0.056754 \pm 0.02115	0 -66 -66 -51 100

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Covariance Matrices

- Do not stand alone
- Are associated with some set of measured or calculated values

Two major categories:

- Covariance matrix associated with experimental data
- Covariance matrix associated with parameters of the theory

Data covariances

Obtaining resonance parameters is a multi-step process:

- 1. Data acquisition** = experimental measurement
- 2. Data reduction** = process of converting from “counts per time-channel” to “cross section”
- 3. Data analysis** = process of parameterizing the cross section in terms of R-matrix theory

- Generally the experimentalist who made the measurement takes care of step 2, the evaluator takes care of step 3.
- However, the two processes are not nearly as independent as the definition would suggest. A simple example is Doppler-broadening, which is always (?) left for the evaluator to include.
- The data covariance matrix provides the linkage between those processes.

Types of data uncertainties

- **Experimentalists define two types of uncertainties**
 - **Statistical** **diagonal data covariance**
 - (due to uncertainty in measurement of raw data, generally assumed to be Poisson statistics)
 - **Systematic “Common”** **off-diagonal data covariance**
 - (due to uncertainties in measurement of parameters for data-reduction process)

Data uncertainties, continued

- **Data reduction ...**

- (the process of converting “counts per channel” to something more closely related to “cross section”)

includes such operations as:

- corrections for detector dead time
- normalization by total run time
- conversion from time to energy scale
- subtraction of backgrounds
- dividing sample-in by sample-out counts (if transmission)

- **It is the data-reduction process that leads to off-diagonal data covariance matrix elements.**

- (Raw data are mutually independent, hence the covariance matrix is diagonal.)

Example of data reduction and error propagation (normalization and background)

- Measure “raw counts” K_i = number of times a neutron was counted in time-channel i .
- Uncertainty on K_i is $\Delta K_i = \sqrt{K_i}$ if Poisson
- Actual “datum” is $D_i = a K_i + b$
 - = reduced data
 - = data that will be analyzed in SAMMYwhere a and b have also been measured, and have uncertainties Δa and Δb respectively.
- Wanted: the uncertainty on D_i and D_j , and the correlation between D_i and D_j

Example, continued

- To find uncertainty and correlation, consider small increments δ for each component:

$$\delta D_i = \delta a K_i + a \delta K_i + \delta b$$

- Square, and take expectation values:

$$\begin{aligned}\langle (\delta D_i \delta D_j) \rangle &= \langle (\delta a K_i + a \delta K_i + \delta b) (\delta a K_j + a \delta K_j + \delta b) \rangle \\ &= \langle (\delta a)^2 \rangle K_i K_j + a^2 \langle (\delta K_i \delta K_j) \rangle + \langle (\delta b)^2 \rangle \\ &= \Delta^2 a K_i K_j + a^2 \Delta^2 K_i \delta_{ij} + \Delta^2 b\end{aligned}$$

This is the data covariance matrix V_{ij}

statistical

systematic due to background

systematic due to normalization

References for data covariances

- **User's Guide to ALEX: Uncertainty Propagation from Raw Data to Final Results for ORELA Transmissions Measurements**
N. M. Larson, ORNL/TM-8676, ENDF-332 (February 1984)
- **Application of New Techniques to ORELA Neutron Transmission Measurements and their Uncertainty Analysis: the Case of Natural Nickel from 2 keV to 20 MeV**
D. C. Larson, N. M. Larson, J. A. Harvey, N. W. Hill, and C. H. Johnson, ORNL/TM-8203, ENDF-333 (October 1983)
- **Uncertainty Propagation from Raw Data to Final Results**
N. M. Larson, *Proceedings of the International Conference on Nuclear Data for Basic and Applied Science, Santa Fe, New Mexico, May 13-17, 1985*, Vol. 2, ed. Phillip G. Young, et al., Gordon and Breach Science Publishers, 1533-1536 (1986)
- **Covariances as Input to and Output from Resonance Analysis**
N. M. Larson, invited paper presented at the International NEANSC Specialists' Meeting on Evaluation and Processing of Covariance Data, Oct 7-9, 1992, held at ORELA at Oak Ridge National Laboratory. Published in *Proceedings of a Specialists' Meeting on Evaluation and Processing of Covariance Data*, ed. M. Wagner 221-238 (1993).
- **Representation and Processing of Covariance Matrices for Resonance Parameters**
N. M. Larson, *Workshop on Covariance Matrices: Generation, Formats, and Applications in Nuclear Energy Technologies*, Brookhaven National Laboratory, 22-23 April 1999.

References for data covariances

- **Practical Alternatives to Explicitly Generating and Inverting Data Covariance Matrices**
N. M. Larson, *Nuclear Mathematical and Computational Sciences: A Century in Review, A Century Anew*, Gatlinburg, Tennessee, April 6-11, 2003, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2003)
- **Some Thoughts on the Data Analysis Process**
Nancy Larson, *Second Research Co-ordination Meeting on Improvement of the Standard Cross Sections for Light Elements, 13-17 October 2003, NIST, Gaithersburg, MD, USA.*
- **Development and Status of Sammy Covariance Generation**
Nancy M. Larson, US DOE NCSP ICSBEP/AROBCAD and ISTC Project 815 Collaborative Meeting, 24-25 November 2003, at ORNL, Oak Ridge, TN, USA.
- **Probability, Statistics, and Data Uncertainties in Nuclear Science and Technology,**
Donald L. Smith, pub. American Nuclear Society, 555 N. Kensington Avenue, LaGrange Park, Illinois 60525 USA (1991)

Compares different methods of treating the data covariance during R-matrix analyses

A good general reference

Concerned with parameter covariance matrix for use in applications work

Other topics related to data covariance ...

(to be discussed later if time permits)

- Comparison of different methods of treating the data covariance information during an R-matrix analysis (file 4x3a.pdf)
- Implicit data covariance matrix (file 4x3b.ppt)

End of “data covariances”

Parameter covariance matrices

- **Reminder:**
 - Covariance matrix does not stand alone, but is always associated with a set of values
- **Initial parameter covariance matrix**
 - Sometimes called “prior”, “á-priori”, ...
 - Is required input for running SAMMY (or any fitting procedure using Bayes’ method)
 - Defaults are provided in the code, but use at your own risk!
 - Often taken to be large and diagonal
 - Least-squares assumption: “large” = “infinite”

Parameter covariance, cont.

- **Output parameter covariance matrix**
 - Sometimes called “final”, “á-posteriori”, ...
 - Generated automatically by SAMMY and most other analysis codes
 - Printed in SAMMY’s LPT file (as uncertainties plus correlation matrix)
 - Stored in COVariance file for use as input for subsequent SAMMY run
 - Can be stored in abbreviated ASCII format

Parameter covariance, cont.

- **Output parameter covariance matrix...**
 - Is needed for calculating uncertainties on derived quantities (k-effective, etc)
 - Can be stored in ENDF file32
 - Major efforts are underway to insert this information
 - Format additions have been adopted for storing very large matrices (LCOMP=2)

End of “parameter covariance matrix”

Covariances for multigroup cross sections

- Used extensively for the first time by Herve Derrien et al.:
Covariance Matrices for Use in Criticality Safety Predictability Studies; ORNL/TM-13492, September 1997
- Procedure:
 - fit differential & integral data → generate values and covariances for resonance parameters
 - calculate differential cross sections with those parameter values; integrate numerically to give group cross sections and covariance matrices

Example: ^{235}U 89 resonances in 0 to 50 eV

Parameters for first seven J=3 resonances:

*****NEW VALUES FOR RESONANCE PARAMETERS

ENERGY (EV)	GAMMA-		GAMMA-		GAMMA-	
	GAMMA	GAMMA	CHANNEL 1	CHANNEL 2	CHANNEL 3	
	L=0 SPIN= 3.0	L=0 SPIN= 0.0	L=0 SPIN= 0.0	L=0 SPIN= 0.0		
3.01247E-01(1)	4.0422E+01(2)	4.7777E-03(3)	1.2256E+02(4)	2.2049E-01(5)		
2.03586E+00(6)	3.7310E+01(7)	9.1821E-03(8)	-1.0168E+01(9)	8.0360E-01(10)		
3.14379E+00(11)	3.8108E+01(12)	2.5643E-02(13)	-2.1236E+01(14)	8.7458E+01(15)		
6.18423E+00(16)	5.4780E+01(17)	7.0752E-02(18)	-4.1715E+01(19)	1.6535E+02(20)		
7.65320E+00(21)	5.7182E+01(22)	3.4280E-03(23)	5.9150E+01(24)	1.0897E+02(25)		
8.88961E+00(26)	4.9288E+01(27)	1.4995E-01(28)	-2.1569E+02(29)	1.3539E+02(30)		
9.71692E+00(31)	4.2720E+01(32)	3.9741E-02(33)	-3.9670E+00(34)	-2.1020E+02(35)		
.						
.						
.						

Example, continued

Absolute and relative uncertainties and correlation matrix for first seven J=3 resonances

	Absolute Uncertainty	Relative Unc.		Correlations														
				1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	4.6545E-04	.002	100															
2	0.8939	.022	-6	100														
3	3.6718E-05	.008	25	51	100													
4	1.255	.010	41	-57	-5	100												
5	2.0350E-02	.092	15	-4	7	-1	100											
6	1.6199E-04	.000	2	-1	0	3	1	100										
7	0.3718	.010	1	1	-3	0	-1	2	100									
8	6.1601E-05	.007	2	3	50	0	1	2	-23	100								
9	0.2398	.024	-9	-1	-1	2	3	-16	-20	-10	100							
10	5.5672E-02	.069	23	-1	0	1	-3	39	-5	3	-3	100						
11	4.1068E-04	.000	7	0	1	2	-1	-3	-3	-1	-6	3	100					
12	0.6285	.016	0	3	0	-1	-1	1	3	0	-4	2	6	100				
13	1.6094E-04	.006	1	2	51	2	2	3	-1	57	-2	2	-17	9	100			
14	0.9287	.044	-26	1	-6	-3	4	6	3	-4	11	-30	-61	-16	8	100		
15	1.175	.013	21	-2	3	5	-2	-1	-3	1	-7	26	22	-22	8	-53	100	
16	1.5426E-03	.000	-2	1	-1	0	1	3	0	-2	0	-3	10	1	-2	4	-5	
17	2.177	.040	-1	1	0	-1	0	0	2	1	-1	-2	2	3	1	0	-2	
18	1.0838E-03	.015	-5	1	19	0	2	2	-1	22	1	-8	4	1	24	7	-7	
19	2.443	.059	-26	2	-5	-5	5	1	-1	-3	8	-32	-2	2	-2	29	-26	
20	3.073	.019	15	-2	0	3	-3	0	0	-1	-3	21	-1	-2	1	-15	18	
21	4.8203E-03	.001	7	0	-2	2	-1	0	-2	-3	1	-3	2	-1	-4	8	-8	

Example, continued

Absolute and relative uncertainties and correlation matrix for first seven J=3 resonances, continued

22	4.292	.075	1	0	-1	0	0	0	1	-1	0	-1	1	1	-1	2	-3
23	1.4500E-04	.042	-10	1	5	-3	2	1	0	5	0	-3	2	1	8	2	-1
24	5.431	.092	-3	-1	0	-2	0	-1	0	-1	-1	3	4	0	-3	-4	2
25	8.324	.076	0	0	0	0	0	2	-1	-1	0	0	-3	0	2	2	1
26	7.7058E-03	.001	13	-1	2	3	-3	-2	2	2	-2	14	-2	0	3	-9	10
27	3.446	.070	-5	1	0	-1	2	1	0	-1	0	-8	2	1	-1	5	-6
28	5.1809E-03	.035	-20	2	5	-3	6	4	-4	6	4	-25	10	1	6	20	-22
29	9.069	.042	-29	2	-1	-7	5	0	-1	2	4	-20	0	1	1	13	-13
30	7.272	.054	6	0	-4	2	0	0	-2	-4	0	-2	0	0	-4	6	-4
31	2.0991E-03	.000	0	0	-2	1	1	1	-2	-2	1	-4	4	0	-2	5	-5
32	2.413	.056	0	0	0	0	0	0	1	0	-1	0	1	2	-1	0	-1
33	8.5402E-04	.021	13	-1	15	3	-2	-1	1	16	-4	16	-7	0	19	-15	16
34	0.3810	.096	-1	0	0	0	0	1	0	0	0	-1	1	0	1	1	-1
35	5.252	.025	6	-1	1	2	-2	-1	1	0	-2	10	-9	-1	3	-9	13

Example, continued

Absolute and relative uncertainties and correlation matrix for first seven J=3 resonances, continued

		16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	
17	2.177	.040	48	100													
18	1.0838E-03	.015	76	39	100												
19	2.443	.059	-24	-8	0	100											
20	3.073	.019	16	-34	24	-59	100										
21	4.8203E-03	.001	-9	0	-8	29	-26	100									
22	4.292	.075	1	0	-1	2	-2	-9	100								
23	1.4500E-04	.042	2	-2	0	-16	8	-46	22	100							
24	5.431	.092	5	-1	-5	-6	-1	14	-5	22	100						
25	8.324	.076	-12	-1	-2	5	-3	-6	-11	36	-30	100					
26	7.7058E-03	.001	2	-3	-1	-26	19	-9	-3	0	1	4	100				
27	3.446	.070	2	2	3	9	-7	2	-2	3	1	1	-19	100			
28	5.1809E-03	.035	6	3	4	31	-30	9	3	10	6	-3	-54	35	100		
29	9.069	.042	6	3	6	12	-7	-29	-1	28	7	0	-4	-1	12	100	
30	7.272	.054	-10	0	-4	18	-14	40	7	-15	-4	-2	-20	2	4	-31	100
31	2.0991E-03	.000	2	0	2	10	-7	21	4	2	-4	14	-4	5	24	-11	54
32	2.413	.056	2	1	0	-1	0	0	0	0	0	0	7	-14	-3	2	-3
33	8.5402E-04	.021	-9	-1	4	-21	17	5	-1	-9	2	-2	-10	-3	-26	-52	29
34	0.3810	.096	2	0	1	-2	1	2	1	3	0	2	5	-2	1	-15	14
35	5.252	.025	-10	-1	0	-13	15	-2	0	-8	0	-7	-13	8	-20	-30	23
		31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	
32	2.413	.056	3	100													
33	8.5402E-04	.021	-17	10	100												
34	0.3810	.096	-23	-1	0	100											
35	5.252	.025	-24	-34	73	-7	100										

Example, continued

Group-averaged capture cross section

Averaged capture cross sections and uncertainties for the lowest 45 groups of the 199-group structure of the VITAMIN-B6 library. Energy boundaries of the groups are given in eV and the cross sections in barns.

	E-min	E-max	theory	uncertainty
(1)	.00001	.00050	1583.62	2.19118
(2)	.00050	.00200	581.447	.814407
(3)	.00200	.00500	332.593	.479974
(4)	.00500	.01000	217.260	.332767
(5)	.01000	.01450	160.512	.265833
(6)	.01450	.02100	126.564	.229096
(7)	.02100	.03000	99.1694	.201790
(8)	.03000	.04000	79.6855	.184531
(9)	.04000	.05000	67.0371	.175575
(10)	.05000	.07000	55.4726	.171735
(11)	.07000	.10000	44.5069	.178960
(12)	.10000	.12500	37.9880	.200970
(13)	.12500	.15000	34.9931	.235094
(14)	.15000	.18400	33.9773	.298876
(15)	.18400	.22500	36.2010	.432866
(16)	.22500	.27500	42.6642	.671274
(17)	.27500	.32500	41.2566	.722969
(18)	.32500	.36680	29.1536	.459712

Example, continued

Group-averaged capture cross section, continued

	E-min	E-max	theory	uncertainty
(19)	.36680	.41399	20.2983	.253470
(20)	.41399	.50000	14.0817	.118298
(21)	.50000	.53158	11.2708	6.544099E-02
(22)	.53158	.62506	9.70383	4.212451E-02
(23)	.62506	.68256	8.48628	2.794191E-02
(24)	.68256	.80000	7.75934	2.375308E-02
(25)	.80000	.87643	7.55463	2.912808E-02
(26)	.87643	1.00000	8.73944	5.500305E-02
(27)	1.00000	1.04000	12.0877	.111810
(28)	1.04000	1.08000	16.3936	.180070
(29)	1.08000	1.12530	24.2145	.299789
(30)	1.12530	1.30000	20.2525	.222470
(31)	1.30000	1.44500	6.60897	8.043458E-02
(32)	1.44500	1.85540	3.84365	1.096020E-02
(33)	1.85540	2.38240	13.3112	8.596037E-02
(34)	2.38240	3.05900	3.56924	3.195349E-02
(35)	3.05900	3.92790	16.2886	.124316
(36)	3.92790	5.04350	21.0874	.123322
(37)	5.04350	6.47600	46.5651	.244552
(38)	6.47600	8.31530	16.2042	8.814033E-02
(39)	8.31530	10.67700	34.4581	.192407
(40)	10.67700	13.71000	67.3420	.253481
(41)	13.71000	17.60400	17.4441	8.699141E-02
(42)	17.60400	22.60300	43.7486	.193572
(43)	22.60300	29.02300	20.0091	.109174
(44)	29.02300	37.26600	34.8962	.157284
(45)	37.26600	47.85100	17.3388	8.418739E-02

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Example, continued

Uncertainties and correlations for group-averaged capture cross sections

Correlation matrix of the capture cross sections for the lowest 45 groups of the 199-group structure of the VITAMIN-B6 library. Absolute errors are given in column 2 of the table, and the correlation coefficients ($\times 100$) follow.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	2.19118	100													
2	.814407	100	100												
3	.479974	100	100	100											
4	.332767	100	100	100	100										
5	.265833	100	100	100	100	100									
6	.229096	100	100	100	100	100	100								
7	.201790	99	99	99	100	100	100	100							
8	.184531	99	99	99	99	100	100	100	100						
9	.175575	99	99	99	99	100	100	100	100	100					
10	.171735	99	99	99	99	99	100	100	100	100	100				
11	.178960	98	98	98	99	99	99	100	100	100	100	100			
12	.200970	98	98	98	98	99	99	99	100	100	100	100	100		
13	.235094	97	97	98	98	98	99	99	99	99	100	100	100	100	
14	.298876	97	97	97	97	98	98	98	99	99	99	100	100	100	100
15	.432866	95	95	95	95	96	96	96	97	97	97	98	98	99	99
16	.671274	90	90	90	91	91	91	92	92	92	93	93	94	95	96
17	.722969	88	88	89	89	89	89	90	90	90	90	91	91	92	93
18	.459712	92	92	92	92	93	93	93	93	93	93	93	93	93	93
19	.253470	94	94	94	94	95	95	95	95	95	95	95	95	94	93
20	.118298	95	95	96	96	96	96	97	97	97	97	96	96	95	93

Note the large off-diagonal correlations

Example, continued

Uncertainties and correlations, continued

21	6.544099E-02	96	96	96	96	97	97	97	97	97	97	97	97	96	96	95	92
22	4.212451E-02	95	95	95	96	96	96	96	96	96	96	96	96	95	94	93	91
23	2.794191E-02	90	90	90	90	90	91	91	91	90	90	89	89	88	86	84	
24	2.375308E-02	72	72	72	73	73	73	73	72	72	72	71	70	69	68	65	
25	2.912808E-02	45	45	45	45	45	45	45	45	44	44	43	42	41	40	38	
26	5.500305E-02	24	24	24	24	24	24	24	24	24	23	22	21	21	20	18	
27	.111810	16	16	16	16	16	16	16	16	16	15	15	14	13	12	11	
28	.180070	13	13	13	13	13	13	13	13	13	13	12	12	11	10	10	
29	.299789	11	11	11	11	11	11	11	12	11	11	11	10	10	9	8	
30	.222470	13	13	13	13	13	13	12	12	12	11	10	10	9	8	8	
31	8.043458E-02	8	8	8	7	7	7	7	6	6	6	6	6	5	5	5	
32	1.096020E-02	24	24	24	24	24	24	24	23	23	22	21	20	19	18	17	
33	8.596037E-02	7	7	6	6	6	6	6	6	6	6	6	5	5	5	5	
34	3.195349E-02	8	8	8	8	8	8	7	7	7	7	7	6	6	6	6	
35	.124316	8	8	8	8	8	8	8	8	7	7	7	7	7	7	6	
36	.123322	3	3	3	3	3	3	3	2	2	2	2	2	2	2	2	
37	.244552	4	4	4	4	4	4	4	4	4	4	3	3	3	3	2	
38	8.814033E-02	4	4	4	4	4	4	4	4	3	3	3	3	3	2	2	
39	.192407	5	5	5	5	5	5	5	4	4	4	4	3	3	3	2	
40	.253481	5	5	5	5	5	5	5	5	4	4	4	4	3	3	3	
41	8.699141E-02	3	3	3	3	3	3	3	3	3	3	3	2	2	2	2	
42	.193572	4	4	4	4	4	4	4	4	4	4	4	3	3	3	2	
43	.109174	2	2	2	2	2	2	2	2	2	2	2	2	2	1	1	
44	.157284	4	4	4	4	4	4	4	4	4	4	3	3	3	2	2	
45	8.418739E-02	2	2	2	2	2	2	2	2	2	2	2	2	1	1	1	

Example, continued

Uncertainties and correlations, continued

		16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
16	.671274	100														
17	.722969	98	100													
18	.459712	94	98	100												
19	.253470	92	95	99	100											
20	.118298	90	93	98	100	100										
21	6.544099E-02	89	91	96	99	100	100									
22	4.212451E-02	87	89	94	97	98	99	100								
23	2.794191E-02	80	82	87	90	92	95	98	100							
24	2.375308E-02	62	63	68	70	74	78	85	94	100						
25	2.912808E-02	36	37	40	42	46	52	61	76	94	100					
26	5.500305E-02	17	18	20	22	25	32	41	60	83	97	100				
27	.111810	10	11	12	14	18	24	33	52	76	93	99	100			
28	.180070	9	9	10	12	15	21	30	48	71	88	96	99	100		
29	.299789	8	8	8	10	13	18	26	42	63	79	87	92	97	100	
30	.222470	7	8	8	9	12	17	24	39	57	69	71	72	73	79	100
31	8.043458E-02	4	4	5	5	7	9	12	19	26	31	33	35	36	37	15
32	1.096020E-02	16	17	18	20	23	29	37	53	71	80	79	74	70	64	64
33	8.596037E-02	5	6	6	6	7	8	9	11	13	14	13	12	11	10	10
34	3.195349E-02	5	4	4	4	5	7	9	12	16	17	16	15	15	15	13
35	.124316	6	6	6	6	7	8	10	14	17	18	16	15	15	15	14
36	.123322	1	2	2	2	2	3	4	6	8	9	8	8	8	8	7
37	.244552	2	2	3	3	4	5	7	9	12	13	12	12	12	11	11
38	8.814033E-02	2	2	2	3	3	4	6	9	11	12	11	11	11	11	11
39	.192407	2	3	3	3	4	6	8	11	15	16	15	14	14	13	13
40	.253481	3	3	3	3	4	6	8	11	15	16	15	15	15	15	14
41	8.699141E-02	2	2	2	2	3	4	6	8	11	11	11	10	10	10	9
42	.193572	2	2	3	3	4	5	7	10	14	15	14	14	14	13	13
43	.109174	1	1	2	2	2	3	4	6	8	9	8	8	8	8	8
44	.157284	2	2	2	3	3	5	6	9	12	13	13	12	12	12	11
45	8.418739E-02	1	1	1	2	2	3	4	6	8	9	8	8	8	8	8

In general, it would be dangerous to ignore such large correlations!

		31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
31	8.043458E-02	100														
32	1.096020E-02	54	100													
33	8.596037E-02	6	33	100												
34	3.195349E-02	9	28	10	100											
35	.124316	8	25	11	30	100										
36	.123322	3	11	7	6	12	100									
37	.244552	5	17	9	8	15	17	100								
38	8.814033E-02	5	16	9	9	16	15	26	100							
39	.192407	6	20	11	11	20	19	28	30	100						
40	.253481	5	20	13	10	22	23	34	30	43	100					
41	8.699141E-02	4	15	9	8	16	15	23	22	30	34	100				
42	.193572	5	19	12	10	21	21	32	29	41	48	34	100			
43	.109174	3	12	8	7	15	14	21	20	28	32	25	33	100		
44	.157284	4	17	11	8	19	19	29	26	38	45	31	43	31	100	
45	8.418739E-02	3	12	8	7	16	14	22	21	30	35	27	35	28	35	100

Multigroup covariances

- What's the point of looking at all these numbers?
- High correlations → possible large effect on calculations of uncertainties on integral quantities
 - for reactor calculations
 - for shielding calculations
 - etc

Communicating the resonance-parameter covariance matrix

- **Resonance parameters**
 - are generated in analysis codes
 - SAMMY etc
 - are communicated via the evaluated nuclear data files
 - ENDF, JENDL, FENDL, BROND, etc.
 - are read and organized in processor codes
 - AMPX, NJOY, PREPRO etc.
 - are used in transport codes, reactor codes, etc.
 - MCNP etc
- **Resonance covariance matrix**
 - must follow the same path

Communicating the cov mtrx, continued

- ENDF formats exist for resonance parameter covariance matrices
 - File 32, LCOMP = 1
 - Can be used for communicating complete covariance matrix for most nuclides
 - Assume “long-range” = 0, everything is “short-range”
 - For the few nuclides where there are “too many numbers”, a new “compact” format was approved at November 2004 meeting LCOMP=2
 - Stores uncertainties plus abbreviated correlation matrix

Communicating the cov mtrx, continued

- Example of “the few nuclides with too many numbers” = ^{235}U
 - 3193 resonances
 - five parameters per resonance
 - 15965 parameters total.
 - number of elements in (half of) covariance matrix = $(15965 \times 15966)/2 = 127,448,595$ elements
 - at six numbers per line, → 21,241,433 lines

The other half of the problem...

- In order to use make use of the covariance matrix in processor codes (etc.), sensitivity coefficients (partial derivatives) are required
 - (SAMMY can generate these, but SAMMY cannot do other things processor codes do)
 - Processor codes are being updated to generate sensitivity coefficients
 - AMPX, NJOY, etc
 - SAMRML code is available for a template
 - written by NML, reads ENDF files and generates cross sections (including angular distributions) and partial derivatives

End of “fitting procedure”