united nations
educational, scientific
and cultural
organization

international atomic
energy agency

the
abdus salam
international centre for theoretical physics

ICTP 40th Anniversary

SMR.1555 - 31

Workshop on
Nuclear Reaction Data and Nuclear Reactors:
Physics, Design and Safety

16 February - 12 March 2004

Further on SAMMY (II)

Nancy M. LARSON
Oak Ridge National Laboratory
Building 5700 MS 6171
P.O. Box 2008
TN 37831-6171 Oak Ridge
U.S.A.

These are preliminary lecture notes, intended only for distribution to participants

SAMMY Workshop

Workshop on Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety

(16 February - 12 March 2004)

Dr. Nancy M. Larson
Oak Ridge National Laboratory

Part 4.3, Fitting Procedure

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 page 3 *ff* in SAMMY Users' Manual**
- **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

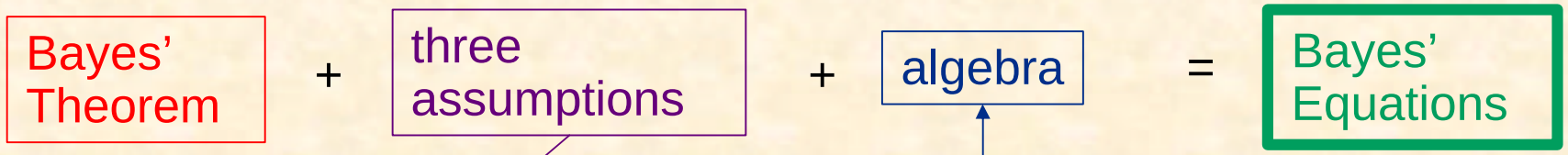
$p(P|B)$ **= prior pdf for the parameters**

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

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

= maximum likelihood function

Bayes' Equations, cont.



- **Assumptions**
  - **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.**
- **Derivation**
  - **Given in the users' guide**
  - **Results only will be shown here**

Not one of these assumptions is true …

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

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

Bayes' Equations (explicitly)

$$P' = P + M'\boxed{Y} \qquad M' = (M^{-1} + \boxed{W})^{-1}$$

$$\boxed{Y} = G^{t} V^{-1} (D - T) \qquad \boxed{W} = G^{t} V^{-1} G$$

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
$P' = P + M' Y$ $\quad M' = (M^{-1} + W)^{-1}$ $Y = G^t V^{-1} (D - T)$ $\quad W = G^t V^{-1} G$	$M' = W^{-1}$
M = initial covariance matrix for parameters	M = infinite, "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

$$C_{ij} = \langle dP_i\, dP_j \rangle = ?P_i\, c_{ij}\, ?P_j$$

where

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

$?P_i$ **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 :**

  $-1 = c_{ij} = +1$

  Also always $|C_{ij}| = ?P_i\, ?P_j$

Why bother with covariances?

- **Integral Quantities are needed for reactor applications**

$$\int_{Emin}^{Emax} s(E)\, j(E)\, dE$$

where

  - **f (E) can be flux or any other function**
  - **s (E) is cross section, calculated from resonance parameters**
  - ***Emin* to *Emax* 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

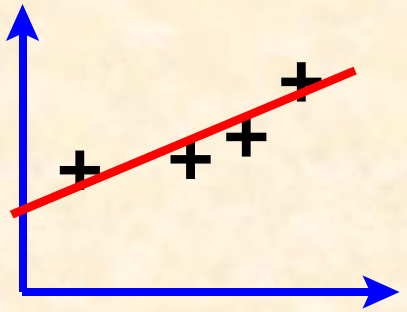
- Suppose a "data fitting program" has found values, uncertainties, and correlation for *a* and *b*. That is,

$< a > = A$ $\quad < (\mathrm{d}a)^2 > = ?^2 A$

$< b > = B$ $\quad < (\mathrm{d}b)^2 > = ?^2 B$

$< \mathrm{d}a\ \mathrm{d}b > = ?A\ ?B\ \ c$

$s(E) = a\,E + b$



(*c* is the correlation coefficient between *A* and *B*)

Example: straight line, continued

- Then suppose the integral quantity of interest is

$$y = \frac{1}{Emax - Emin} \int_{Emin}^{Emax} s(E)\,dE = \frac{1}{Emax - Emin} \int_{Emin}^{Emax} (aE + b)\,dE$$

$$= \frac{1}{Emax - Emin} \left(a \frac{Emax^2 - Emin^2}{2} + b(Emax - Emin) \right)$$

$$= ae + b$$

where e is the midpoint of the range, e = (*Emax*-*Emin*)/2

Example: straight line, continued

- Expected value of *y* is $Y = (Ae+B)$. What is uncertainty on *Y* ?
- Uncertainties are "propagated" by taking small increments, squaring, and taking expectation values.

$$dy = d\boldsymbol{a}\, e \;+\; d\boldsymbol{b}$$

$$\left\langle (dy)^2 \right\rangle = \left\langle (d\boldsymbol{a}\, e + d\boldsymbol{b})^2 \right\rangle$$

$$= \left\langle (d\boldsymbol{a})^2 \right\rangle e^2 + 2\left\langle d\boldsymbol{a}\, d\boldsymbol{b} \right\rangle e + \left\langle (d\boldsymbol{b})^2 \right\rangle$$

- Rewriting this gives

$$\Delta^2 \boldsymbol{Y} = e^2\, \Delta^2 \boldsymbol{A} \;+\; 2e\, \boldsymbol{c}\, \Delta \boldsymbol{A}\, \Delta \boldsymbol{B} \;+\; \Delta^2 \boldsymbol{B}$$

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

Example: straight line, continued

- **TRY SOME NUMBERS...**

  A **= 100±10,** ***B*** **=40±5,** ***Emin*** **= 0.5,** ***Emax*** **= 1.5 so e = 1.0**

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

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

c = 0 implies ? *Y* = 11.18

c = 1 implies ? *Y* = 15.00

c = - 1 implies ? *Y* = 5.00

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

Therefore Y ± ? *Y* = 140.00 ± 5.00 if *c* = -1

= 140.00 ± 11.18 if *c* = 0

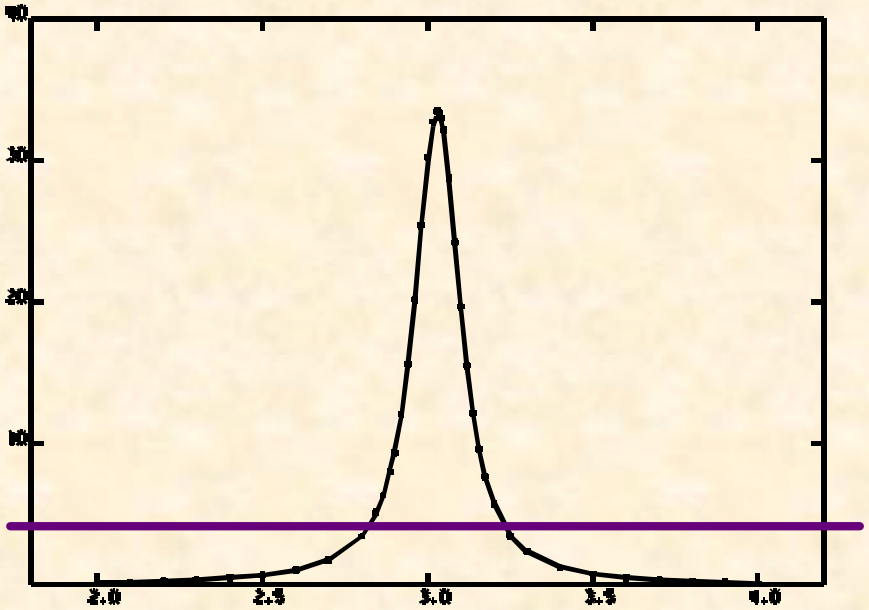
= 140.00 ± 15.00 if *c* = 1

Unc ~ 4 %

Unc ~ 8 %

Unc ~11 %

More realistic example

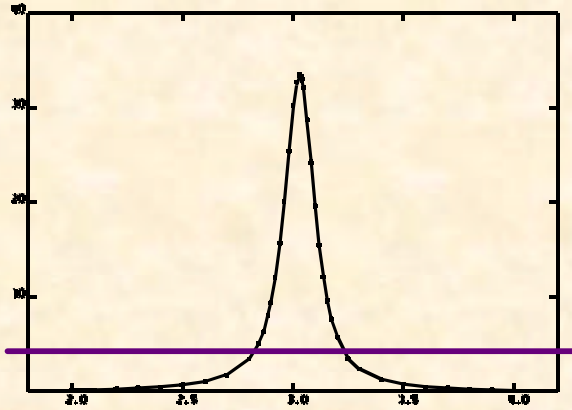


Wanted: to find the average value of this cross section

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	±	0.00006	100
$G_?$	0.051323	±	0.01952	0 100
G_n	0.0000218	±	0.0000044	0 100 100
G_{f1}	-0.036825	±	0.01720	0 -31 -31 100
G_{f2}	0.056754	±	0.02115	0 -66 -66 -51 100

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 $?K_i$** $= \sqrt{K_i}$ **if Poisson**
- **Actual "datum" is $D_i = a\,K_i + b$**

  = reduced data
  = data that will be analyzed in SAMMY

  where *a* and *b* have also been measured, and have uncertainties $?a$ and $?b$ 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 d for each component:**

$$dD_i = da\,K_i + a\,dK_i + db$$

- **Square, and take expectation values:**

$$\begin{aligned}\left\langle (dD_i dD_j) \right\rangle &= \left\langle \left(d\,\boldsymbol{a}\,\boldsymbol{K}_i + \boldsymbol{a}\,d\,\boldsymbol{K}_i + d\,\boldsymbol{b}\right)\left(d\,\boldsymbol{a}\,\boldsymbol{K}_j + \boldsymbol{a}\,d\,\boldsymbol{K}_j + d\,\boldsymbol{b}\right)\right\rangle \\ &= \left\langle (d\,\boldsymbol{a})^2 \right\rangle \boldsymbol{K}_i\,\boldsymbol{K}_j + \boldsymbol{a}^2 \left\langle \left(d\,\boldsymbol{K}_i\,d\,\boldsymbol{K}_j\right) \right\rangle + \left\langle (d\,\boldsymbol{b})^2 \right\rangle \\ &= \Delta^2 \boldsymbol{a}\,\boldsymbol{K}_i\,\boldsymbol{K}_j + \boldsymbol{a}^2\,\Delta^2 \boldsymbol{K}_i\,d_{ij} + \Delta^2 \boldsymbol{b}\end{aligned}$$

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 815Collaborative 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

SPIN GROUP NUMBER 1  WITH SPIN= 3.0, ABUNDANCE= 1.0000, AND G*ABNDNC= .4375
                  "true" radius =  9.0000E+00       9.0000E+00       9.0000E+00
               effective radius =  9.6566E+00       9.6566E+00       9.6566E+00
    ENERGY          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
     (EV)          (MILLI-EV)       (MILLI-EV)       (MILLI-EV)       (MILLI-EV)
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	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

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 (×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	99	100	100	100	
15	.432866	95	95	95	95	96	96	96	97	97	97	98	98	99	99	100
16	.671274	90	90	90	91	91	91	92	92	92	93	93	94	95	96	98
17	.722969	88	88	89	89	89	89	90	90	90	90	91	91	92	93	95
18	.459712	92	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	95	94	93
20	.118298	95	95	96	96	96	96	97	97	97	97	96	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	96	96	95	92
22	4.212451E-02	95	95	95	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	2	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	2	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 provisionally approved at November 2003 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 = (15965×15966)/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"

SAMMY Workshop

Workshop on Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety

(16 February - 12 March 2004)

Dr. Nancy M. Larson
Oak Ridge National Laboratory

Part 7. Miscellaneous topics

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

Auxiliary codes

- **angodf**
  - **translate differential elastic data plot file from "a function of energy for a given angle" to "a function of angle for a given energy"**
- **convrt**
  - **convert from REFIT input to SAMMY or vice versa (resonance parameters only)**
- **samamr**
  - **rearrange data-reduction parameters when analyzing data sets sequentially**
- **samamx**
  - **modify the value of one non-varied resonance parameter (to be used with extreme caution)**

Auxiliary codes, continued

- **samcpr**
  - **provide direct comparison of results of calculations from two codes**
    - **the "other" code results are used as "experimental data" for SAMMY runs, to give both calculations at the exact same energies**
- **samdis**

More on this later…

  - **calculate statistical properties after completion of an analysis**
- **samftz**
  - **adjust tzero and L for an experimental data set**

Auxiliary codes, continued

- **samort**
  - **generate plots of ORR resolution broadening function (and/or pieces thereof) with respect to energy or time-of-flight**
- **samplt** More on this later…
  - **alternative method for generating plot files**
- **samqua**
  - **generate quantum numbers for spin groups (recently generalized by Olivier Bouland, Richard Babut, and Nancy Larson)**

Already discussed

Auxiliary codes, continued

- **samrpt**
  - **generate plots of RPI resolution broadening function (and/or pieces thereof) with respect to energy or time-of-flight**
- **samrst**
  - **generate plots of original (RSL) resolution broadening function (and/or pieces thereof) with respect to energy or time-of-flight**
- **samsmc**
  - **perform Monte Carlo simulations of multiple-scattering corrections for capture or fission, to ensure consistency with SAMMY results**
- **samsta**
  - **generate staircase plots of resonances**

Auxiliary codes, continued

- **samthn**
  - **thin dense experimental data by averaging over a specified number of points in a given energy range**
- **suggel**
  - **suggest values for *l* and *J* for a given resonance (written by S. Y. Oh and L. C. Leal, not completely portable)**
- **samrml**
  - **read ENDF file 32 LRF=7 and generate cross sections (including angular distributions) and partial derivatives**
  - **intended as prototype for processor codes**

Auxiliary codes, continued (plotting)

- **forodf**
  - **ORELA code for manipulating & plotting results**
  - **very old, not maintained, not portable**
  - **is used for this workshop**
- **rsap**
  - **more modern code for plotting results**
  - **contains helpful preprocessor features**
  - **under development (Royce Sayer at ORNL)**
  - **not yet portable, not released**

Plotting

- **What to do on your own computers if you do not have forodf or rsap?**
- **SAMMY provides two kinds of files from which plots can be made**
  - **SAMMY.ODF (ORELA Data Format; single-precision)**
  - **SAMMY.PLT (binary format; double-precision)**
- **Auxiliary program samplt was designed to read SAMMY.PLT and rewrite in other format**
  - **Users can redesign the output from samplt as needed for your own plotting package, by modifying the FORTRAN**

Program samdis

- **modified version of SAMDIST, written by Luiz Leal**
- **used to verify consistency of resonance parameter set with predicted theoretical statistical distribution.**

- **Reference**
  - **“SAMDIST: A Computer Code for Calculating Statistical Distributions for R-Matrix Resonance Parameters”, L. C. Leal & N. M. Larson, ORNL/TM-13092 (September 1995)**
  - **Also see SAMMY users’ manual (pages 150z.5-6) for update**

Program samdis, continued

- **Three statistical tests (details are given in samdist manual)**
  1. **Level spacing distributions are compared with the Wigner distribution law**
  2. **Neutron, radiation, and fission width distributions are calculated and compared with the ?2 distribution with the appropriate number of degrees of freedom –**
     - **dof = 1 for the Porter-Thomas distribution of neutron widths**
     - **dof = 2 or 3 for fission**
     - **dof = 8 for capture widths**
  3. **Long-range correlations of the energies are tested via the ?3 statistic of Mehta and Dyson**

Other SAMMY features worth noting

- **ENDF file 2 (isotopic) can be used for initial PAR file.**
  - **LRF=1,2,3,7**
- **SAMMY can report results in ENDF file 2 format**
  - **LRF=1,2 (Breit-Wigner)**
  - **LRF=3 (so-called Reich-Moore)**
  - **LRF=7 (new R-Matrix Limited)** ← **Recommended for all future work**
- **SAMMY is not confined to ENDF File 2 RM format limitations!**
  - **Spin-group-dependent radii; channel-dependent radii**
  - **As many entrance and/or exit channels as needed for a given Jp**
  - **Coulomb penetrabilities if needed**

Other features, continued

- **Wanted: cross section as a function of energy for a given set of resonance parameters. Unavailable: experimental data to specify the energy grid. What to do?**
  1. **Use any available energy grid, or generate a "dummy" grid, in the appropriate energy range. Run SAMMY, ignore the "data" and look only at the "theory".**
  2. **If things look odd with #1, it may be that the energy grid is inappropriate for this resonance structure. Solution: Pretend you want Doppler (and/or resolution) broadening. This will force SAMMY to generate an auxiliary grid (which *will* be appropriate for the resonance parameters you are using), which can be written to an output file using the command "plot unbroadened cross sections".**
  3. **Alternatively, use the "reconstruct cross section from resonance parameters" command. This command causes SAMMY to generate an energy grid using techniques (and programming) borrowed from NJOY.**

Other features, continued

- **Stellar (Maxwellian) averages can be generated as a function of temperature, for use in nuclear astrophysics applications.**
  - **Covariance matrix is also generated.**

- **Multigroup cross sections can be calculated with**
  - **either (1) no corrections to the theoretical values, or (2) Doppler and/or resolution broadening, multiple-scattering corrections, etc., and**
  - **either Bondarenko narrow resonance scheme or energy- or time-weighted averaging.**
  - **Covariance matrix is automatically generated**

Other features, continued

- **There is no covariance matrix in the evaluated files. What to do?**
  - **SAMMY can retroactively generate an *approximate* covariance matrix for resonance parameters, even after the evaluation is complete.**
    - **Needed – all (or most) of the data used for the original analysis.**
      - **If absolutely necessary, can use SAMMY to "invent" data, then make reasonable assumptions about the uncertainties on those data**
    - **Procedure involves simultaneous fitting (with no iteration) of the available data.**
      - **Underlying assumption is that parameter values will change very little, so covariance matrix is appropriate for the unchanged parameter values.**

Other features, continued

- **Mismatch in energy-scale between two data sets can sometimes be corrected by having SAMMY fit *t* 0 and *L*. Program samftz can then provide modified data file.**
- **Spin-group-dependent detector efficiencies can be used for analysis of capture or fission yields or self-indication data.**
- **Angle-differential reaction cross sections (as well as angle-differential elastic cross sections) can be calculated.**

Other features, continued

- **It is possible to generate a phony theoretical "cross section" which is constant, linear, delta-function, or 1/*v*. These are useful for testing resolution functions, for example.**
- **Information for resolution functions, for normalizations and backgrounds, and for "miscellaneous" parameters can now be in the INPut file instead of the PARameter file, so long as no parameters are to be varied.**
  - **CAUTION: Double-check the LPT file to be sure SAMMY is actually doing what you wanted!**

Very new, not in any released version of the code

Quality assurance

How do we know that SAMMY is doing what it's supposed to be doing?

- **SAMMY QA program involves "test cases"**
- **Each test case is designed to test a particular feature of the code**
- **A new test case is created when**
  - **a new feature is added to SAMMY**
  - **a major bug is exterminated**
- **All test cases are rerun**
  - **after major changes / additions to the code**
  - **prior to each official release**
  - **upon porting to a new computer platform**
  - **whenever the author feels the need**

Quality assurance, continued

- **Test cases (input and output) are released along with source code (from RSICC or NEA), and should be run whenever the code is ported to a new platform --**
  - **to resolve differences**
  - **to find bugs that show up on your system but not on the author's**
  - **to be sure the code you are using behaves properly**
- **NOTE: When porting SAMMY to your computer, run *all* test cases and compare your output to the author's, before beginning to run your own analyses. *At least run those cases which use the features you are using!***
  - **Be sure run the relevant test cases before you contact the author for help.**
- **Another use for test cases -- provide sample input for specific features of the code**
  - **A table in the manual provides a list of all available test cases and which features they pertain to.**

End of miscellaneous topics