Error Propagation, Least-Squares and Weighted Average

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1 Error Propagation

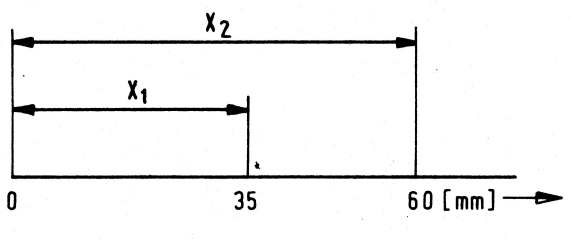
1.1 Basic Formulae

- $\mathrm{d}x = x - \langle x \rangle$
- $\delta x = (x - \langle x \rangle)/\langle x \rangle$
- Variance $V_{xx} = \langle (x - \langle x \rangle)^2 \rangle = \langle \mathrm{d}x \cdot \mathrm{d}x \rangle = \langle x^2 \rangle - \langle x \rangle^2$
- Covariance $V_{xy} = \langle (x - \langle x \rangle)(y - \langle y \rangle) \rangle = \langle \mathrm{d}x \cdot \mathrm{d}y \rangle = \langle xy \rangle - \langle x \rangle \langle y \rangle$
- Standard deviation $\Delta x = \sqrt{V_{xx}}$
- Fractional standard deviation $f_x = \Delta x / \langle x \rangle$
- Fractional covariance $v_{xy} = V_{xy}/(\langle x \rangle \langle y \rangle) = \langle (x - \langle x \rangle)(y - \langle y \rangle) \rangle / (\langle x \rangle \langle y \rangle) = \langle \delta x \cdot \delta y \rangle$
- Correlation coefficient $c_{xy} = V_{xy} / \sqrt{V_{xx} V_{yy}}$
- For linear combination $p = \sum_{i=1}^{n} a_{pi} x_{pi}$ and $q = \sum_{i=1}^{n} a_{qi} x_{qi}$,
  $V_{pq} = \sum_{i,j=1}^{n} a_{pi} a_{qj} V_{ij}$, $V_{pp} = \sum_{i=1}^{n} a_{pi}^2 V_{ii} + 2 \sum_{i=1}^{n} \sum_{j>i}^{n} a_{pi} a_{pj} V_{ij}$,
  where V_{ij} is the covariance between x_{pi} and x_{qj}.
- For product/quotient function $p = \frac{\prod_{k=1}^{m} x_{pk}}{\prod_{k=m+1}^{n} x_{pk}}$ and $q = \frac{\prod_{k=1}^{m} x_{qk}}{\prod_{k=m+1}^{n} x_{qk}}$,
  $v_{pq} \sim \sum_{k=1}^{n} c_{pq,k} f_{x_{pk}} f_{x_{qk}}$, $v_{pp} \sim \sum_{k=1}^{n} f_{x_{pk}}^2$,
  if correlation between x_{pk} and x_{ql} exists only when $k = l$ (correlation coefficient $c_{pq,k}$).
- For general function, $p = (x_{p1}, x_{p2}, ..., x_{pn})$ and $q = (x_{q1}, x_{q2}, ..., x_{qn})$,
  $V_{pq} \sim \sum_{i,j=1}^{n} g_{pi} g_{qj} V_{ij}$, $V_{pp} \sim \sum_{i=1}^{n} g_{pi}^2 V_{ii}$,
  where $g_{pi} = (\partial p / \partial x_{pi})_{x_{pi} = \langle x_{pi} \rangle}$, $g_{qj} = (\partial q / \partial x_{qj})_{x_{qj} = \langle x_{qj} \rangle}$, V_{ij} is the covariance between x_{pi} and x_{qj}.

1.2 Measurement of Lengths by Gauge Blocks [*1]

An experimenter, a "Mr.A.", has to determine two markings on a length scale of distances from a fixed zero point, $x_1 = 35$ mm and $x_2 = 60$ mm (see Fig. 1). For this experiment he uses three gauge blocks of defined

Fig. 1:



length and with well known variances:

Gauge block		Length [mm]	Std.Dev. [μm]	Variance [μm^2]
l_1	=	50	0.05	Var(l_1)=0.0025
l_2	=	15	0.03	Var(l_2)= A1-1
l_3	=	10	0.02	Var(l_3)= A1-2

(A-1)

The first marking is obtained by using the gauge block l_1 and subtracting the length l_2, while the second marking is reached by adding to l_1 the length of l_3, I.e.:

$$\begin{aligned} x_1 &= l_1 - l_2, \\ x_2 &= l_1 + l_3. \end{aligned} \tag{A-2}$$

By using the uncertainty propagation rules:

$$\begin{aligned} \mathrm{Var}(x_1) &= 0.0034, \\ \mathrm{Var}(x_2) &= \boxed{\text{A1-3}}. \end{aligned} \tag{A-3}$$

"Mr.A." states his final result as:

	Std.Dev.	
$x_1 = 35$ mm	A1-4	μm,
$x_2 = 60$ mm	A1-5	μm.

(A-4)

What he has be done appears correct. We will however come back to this point later.

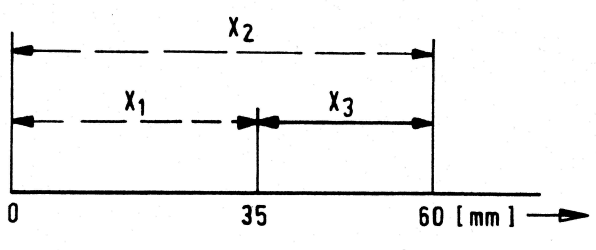
Some time after this experiment one is interested in an additional quantity, x_3, which defines the distance between both markings set by "Mr.A." (see Fig. 2). Two colleagues of "Mr.A.", "Mr.B." and "Mr.C.", are engaged to establishing this new quantity. They proceed using different methods.

"Mr.B." uses the same set of gauge blocks as "Mr.A." and can establish that the distance x_3 can be reproduced by addition of the length of the gauge blocks l_2 and l_3. He obtains

$$\begin{aligned} & x_3 = l_2 + l_3 = 25 \text{ mm}, \\ \text{and} \quad & \\ & \mathrm{Var}(x_3) = \mathrm{Var}(l_2) + \mathrm{Var}(l_3) = \boxed{\text{A1-6}}\ \mu\text{m}^2. \end{aligned} \tag{A-5}$$

[*1] Extraction from Ref. [1] with minor modification.

Fig. 2:



At the same time, “Mr.C.” uses the information given by “Mr.A.” in Eq. (A-2) and (A-3) and calculates:

$$\begin{aligned} & x_3 = x_2 - x_1 = 25 \text{ mm}, \\ \text{and} \quad & \\ & \mathrm{Var}(x_3) = \mathrm{Var}(x_2) + \mathrm{Var}(x_1) = \boxed{\text{A1-7}}\ \mu\text{m}^2. \end{aligned} \tag{A-6}$$

At first glance the situation looks frustrating. The two experimenters “Mr.B.” and “Mr.C.” have both done correct work and obtained the different results of Eq. (A-5) and Eq. (A-6), respectively. What happened? To understand that we have to go back to the first experiment of “Mr.A.”. Looking at Eq. (A-2) we recognize that “Mr.A.” used in both the determination of x_1 as well as x_2 the length of the gauge block l_1. Further, looking at Eq. (A-3) and (A-4), we find that the information of l_1 being common to both x_1 and x_2 was not communicated in the final results, The whole information is only given if we replace Eq. (A-3) by:

$$\begin{aligned} \mathrm{Var}(x_1) &= \mathrm{Var}(l_1) + \mathrm{Var}(l_2), \\ \mathrm{Var}(x_2) &= \mathrm{Var}(l_1) + \mathrm{Var}(l_3), \\ \mathrm{Cov}(x_1, x_2) &= \mathrm{Var}(l_1). \end{aligned} \tag{A-7}$$

The complete covariance matrix (in μm^2) is then:

$$\begin{pmatrix} \mathrm{Var}(x_1) & \mathrm{Cov}(x_2, x_1) \\ \mathrm{Cov}(x_1, x_2) & \mathrm{Var}(x_2) \end{pmatrix} = \begin{pmatrix} 0.0034 & \boxed{\text{A1-8}} \\ \boxed{\text{A1-9}} & \boxed{\text{A1-10}} \end{pmatrix}. \tag{A-8}$$

With this information the final result of Eq. (A-4) should be written:

$$\begin{array}{lll} & \text{Std.Dev.} & \text{Correlation Matrix} \\ x_1 = 35 \text{ mm} & 0.058\ \mu\text{m} & \begin{pmatrix} \boxed{\text{A1-11}} & \boxed{\text{A1-12}} \\ \boxed{\text{A1-13}} & \boxed{\text{A1-14}} \end{pmatrix} \\ x_2 = 60 \text{ mm} & 0.054\ \mu\text{m} & \end{array} \tag{A-9}$$

From Eq. (A-9) we recognize that x_1 and x_2 are not independent since their correlation coefficient is 0.80. Due to the symmetry of the correlation matrix it is in most cases sufficient to state only the upper or lower half of this matrix.

Using this complete information the procedure of “Mr.C.” shown in Eq. (A-6) changes and “Mr.C.” would obtain:

$$\begin{aligned} x_3 &= x_2 - x_1 = 25 \text{ mm}, \\ \text{and} \quad & \\ \mathrm{Var}(x_3) &= \mathrm{Var}(x_2) + \mathrm{Var}(x_1) - 2\,\mathrm{Cov}(x_1, x_2) = \boxed{\text{A1-15}}\ \mu\text{m}^2. \end{aligned} \tag{A-10}$$

1.3 Direct (Absolute) Measurement of Neutron Cross Section [*2]

One of the methods for cross section determination is the activation of defined materials in well-known neutron fields and the subsequent deduction of a cross section σ from the induced radioactivity. The relationship is:

$$\sigma_i = \frac{A_i}{\epsilon_i}\frac{1}{N_i}\frac{1}{\phi_i} \tag{A-11}$$

with i being an index indicating a specific material and type of reaction. A_i is the measured counting rate, N_i is the number of contributing atoms and ϕ_i is the neutron flux density at the position of the probe during the irradiation process. We assume a mono-energetic neutron field of the energy, E_n, so that $\sigma_i = \sigma_i(E_n)$. The efficiency of the detector, ϵ_i, used in measuring the radioactivity depends on the energy of the gamma rays produced in a specific neutron reaction, i.e. $\epsilon_i = \epsilon(E_{\gamma i})$.

We assume that three different reaction cross sections were measured in the same mono-energetic neutron field. i.e., $\phi_1 = \phi_2 = \phi_3$. A complete list of the various components contributing to the uncertainty of Eq. (A-11) of all three experiments is as follows:

Table 1:

Rel.Std.Dev.(in %)			
$i =$	1	2	3
A_i	0.5	1.0	0.3
ϵ_i	1.6[a]	2.2[a]	1.3[a]
ϕ_i	2.0[b]	2.0[b]	2.0[b]

[a]Correlation coefficients: $\mathrm{Cor}(\epsilon_1, \epsilon_2)$=0.8,
$\mathrm{Cor}(\epsilon_1, \epsilon_3)$=0.5,
$\mathrm{Cor}(\epsilon_2, \epsilon_3)$=0.9

[b]Fully correlated (same neutron field !)

The uncertainty contribution from N_i is usually very small and can therefore be neglected. In most cases the various components contributing to the uncertainty of a single experiment (fixed i) can be defined in such a way that there are no correlations between components belonging to the same measurement. We see from Table 1 that no vertical correlations exist only horizontal ones, namely between components belonging to different experiments.

Regarding the quoted correlations in more detail, we observe no correlation between the measured counting rates. This indicates that the uncertainty due to counting statistics dominates all other uncertainty components which may contribute to the total uncertainty of the radioactivity measurement. The particular correlations between the various efficiencies are attributed to the relationship describing the efficiency. The neutron flux density is the same for all three experiments, and so must be taken into account by a correlation coefficient of 1.

Using the definitions

$$\mathrm{d}x_i = x_i - \langle x_i \rangle, \tag{A-12}$$

$$\delta x_i = \mathrm{d}x_i / x_i, \tag{A-13}$$

[*2]Extraction from Ref. [1] with minor modification.

we can express the deviation from the expected value of Eq. (A-11) as

$$\mathrm{d}\sigma_i = \frac{\partial \sigma_i}{\partial A_i}\mathrm{d}A_i + \frac{\partial \sigma_i}{\partial \epsilon_i}\mathrm{d}\epsilon_i + \frac{\partial \sigma_i}{\partial \phi_i}\mathrm{d}\phi_i, \tag{A-14}$$

and therefore we can formally write the relative deviations from the expected values as

$$\delta\sigma_i = \delta A_i - \delta\epsilon_i - \delta\phi_i. \tag{A-15}$$

The estimates of the variances and covariances are given by forming the expected values $\langle \delta\sigma_i \; \delta\sigma_i \rangle$ and $\langle \delta\sigma_i \; \delta\sigma_j \rangle$ respectively, *with due regard* to the signs of Eq. (A-15).

We have no vertical correlations which means that terms of the form of $\langle \delta A_i \; \delta\epsilon_i \rangle$ and $\langle \delta A_i \; \delta\phi_i \rangle$ and $\langle \delta\epsilon_i \; \delta\phi_i \rangle$ do not exist.

With $\langle \delta A_i \; \delta A_j \rangle = 0$, i.e. no correlation between the measured count rates we can immediately write:

$$\begin{array}{lllll} \text{Rel.Var.}(\sigma_i) = & \langle \delta\sigma_i \; \delta\sigma_i \rangle = & \langle \delta A_i \; \delta A_i \rangle + & \langle \delta\epsilon_i \; \delta\epsilon_i \rangle + \langle \delta\phi_i \; \delta\phi_i \rangle, \\ \text{Rel.Cov.}(\sigma_i, \sigma_j) = & \langle \delta\sigma_i \; \delta\sigma_j \rangle = & & \langle \delta\epsilon_i \; \delta\epsilon_j \rangle + \langle \delta\phi_i \; \delta\phi_j \rangle. \end{array} \tag{A-16}$$

The relative covariance matrix (in $\%^2$) is then

$$\begin{array}{ll} i = 1 & \left(\begin{array}{lll} \boxed{\text{A2-1}}^2 + 1.6^2 + 2.0^2 & & \\ \boxed{\text{A2-2}} \times 1.6 \times 2.2 + 2.0^2 & \boxed{\text{A2-3}}^2 + 2.2^2 + 2.0^2 & \\ \boxed{\text{A2-4}} \times 1.6 \times 1.3 + 2.0^2 & \boxed{\text{A2-5}} \times 2.2 \times 1.3 + 2.0^2 & \boxed{\text{A2-6}}^2 + 1.3^2 + 2.0^2 \end{array} \right) \\ i = 2 & \\ i = 3 & \end{array} \tag{A-17}$$

$$= \left(\begin{array}{lll} 6.81 & & \\ 6.82 & 9.84 & \\ 5.04 & 6.57 & 5.78 \end{array} \right).$$

The final result can also be stated as:

Measured quantity	Rel.Std.Dev. %	Correlation Matrix		
σ_1	A2-7	A2-10		
σ_2	A2-8	A2-11	A2-12	
σ_3	A2-9	A2-13	A2-14	A2-15

(A-18)

1.4 Relative Measurement of Neutron Cross Sections [*3]

The example presented here is based on an experiment of Cf-252 spectrum averaged cross sections published by Kobayashi and Kimura [2, 3]. Our example contains a small subset of the complete analysis: the ratio measurement of the ^{27}Al(n,p) cross section relative to the ^{27}Al(n,α) cross section and a ratio measurement of the ^{24}Mg(n,p) cross section relative to the ^{115}In(n,n') cross section. The symbol σ_i stands for the spectrum averaged cross section. The results were:

$$\begin{array}{lcll} \sigma_2\left[^{27}\mathrm{Al(n,p)}\right] & / & \sigma_1\left[^{27}\mathrm{Al(n,}\alpha\mathrm{)}\right] & = 4.797, \\ \sigma_4\left[^{24}\mathrm{Mg(n,p)}\right] & / & \sigma_3\left[^{115}\mathrm{In(n,n')}\right] & = 0.009651. \end{array} \tag{A-19}$$

Using the definition of Eq. (A-11) one can write such ratios as with

$$\sigma_i/\sigma_j = P_i/P_j \tag{A-20}$$

with

$$P_i = \frac{A_i}{\epsilon_i}\frac{1}{N_i}\prod_l k_i^l. \tag{A-21}$$

The product of the k_i^l-terms stands for corrective terms necessary to reduce the measured quantities to the simple form of Eq. (A-11). The complete list of all uncertainty contributions and their correlations is given in Table 2. The principle of such measurements is the parallel irradiation of two different foils in the same neutron field and subsequent counting of the induced radioactivities. The experimentally determined quantities P_i of Eq. (A-21) are terms of the form $\sigma_i\,\phi_i$. The unknown neutron flux density is eliminated by forming the ratio.

Table 2: List of the Uncertainty Components (from Ref. [2])

Uncertainties (in %) due to	Symbol	Run - 1		Run - 2	
		^{27}Al(n,α)	^{27}Al(n,p)	^{115}In(n,n')	^{24}Mg(n,p)
	No.	1	2	3	4
Counting statistics	A_i	1.6	2.0	1.0	3.2
Efficiency	ϵ_i	1.1[a]	1.4[a]	2.2[a]	1.1[a]
Geometrical factor	k_i^G	2.0[b]	2.0[b]	2.0[b]	2.0[b]
Half life	k_i^T	0.2[c]	-	-	0.2[c]
Mass determination	N_i	0.1[d]	0.1[d]	0.1	0.2
Back scattering	k_i^B	0.7[e]	1.0[e]	1.0[e]	0.7[e]
Irradiation and colling time	k_i^H	0.1	1.8	0.1	0.1
Gamma ray attenuation	k_i^S	0.5[f]	0.5	1.0	0.5[f]
Gamma ray intensity	k_i^J	0.1[g]	1.0	1.0	0.1[g]
Others	k_i^R	1.0	1.0	1.0	1.0

a Cor(ϵ_1, ϵ_4) = 1.00, Cor(ϵ_1, ϵ_3) = Cor(ϵ_3, ϵ_4) = 0.80, Cor(ϵ_1, ϵ_2) = Cor(ϵ_2, ϵ_4) = 0.94, Cor(ϵ_2, ϵ_3) = 0.95
b, e Fully correlated
c, f, g Fully correlated (same product nucleus)
d Fully correlated (same foil)

In Table 2 the uncertainties of the A_i are regarded as being independent. I.e., uncertainties due to effects such as the determination of photo-peak area or background subtraction, which would establish correlations, were neglected compared with the counting statistics. The efficiency correlations (a) come from the

[*3] Extraction from Ref. [1] with minor modification.

interpolation procedure used to determine the efficiency (more details on that are given in subsection E.4.2 of [1]). The correction of the geometrical factor is the same for all measurements, and so the corresponding uncertainties show full correlation (b). The uncertainties of the back-scattering correction are different but, as the source of the back-scattering (room walls) is the same, the quantities must be assumed to be fully correlated (e). The measurements no. 1 and no. 2 are based on the mass determination of a common aluminium foil, therefore the correlation is 100% (d).

The product nucleus, ^{24}Na, is the same for both reactions ^{27}Al(n,α) and ^{24}Mg(n,p), therefore all uncertainty components depending on the common radioactive decay, half life and mass attenuation must be fully correlated (c, f-g). Finally one should comment that uncertainty sources should normally be specified better than under the title "Others", as given in Table 2.

We can express the deviation from the expected value of Eq. (A-21) as

$$\mathrm{d}P_i = (\partial P_i)/(\partial A_i)\mathrm{d}A_i + (\partial P_i)/(\partial \epsilon_i)\mathrm{d}\epsilon_i + (\partial P_i)/(\partial N_i)\mathrm{d}N_i + \sum_l (\partial P_i)(\partial k_i^l)\mathrm{d}k_i^l, \tag{A-22}$$

and therefore we can formally write Formally we can write

$$\delta P_i = \delta A_i - \delta\epsilon_i - \delta N_i + \sum_l \delta k_i^l \tag{A-23}$$

As Table 2 shows no vertical correlations, the relative covariance of the measured P_i is

$$\langle \delta P_i\, \delta P_j\rangle = \langle \delta A_i\, \delta A_j\rangle + \langle \delta\epsilon_i\, \delta\epsilon_j\rangle + \langle \delta N_i\, \delta N_j\rangle + \sum_l \langle \delta k_i^l\, \delta k_j^l\rangle, \tag{A-24}$$

i.e. we have no mixed terms between the components of Eq. (A-23).

What we want to determine is the covariance matrix of the ratios

$$\begin{aligned} R_{12} &= P_2/P_1, \\ R_{34} &= P_4/P_3. \end{aligned} \tag{A-25}$$

With

$$\begin{aligned} \delta R_{12} &= \delta P_2 - \delta P_1, \\ \delta R_{34} &= \delta P_4 - \delta P_3, \end{aligned} \tag{A-26}$$

we obtain

$$\begin{aligned} \langle \delta R_{12}\, \delta R_{12}\rangle &= \langle \delta P_2\, \delta P_2\rangle + \langle \delta P_1\, \delta P_1\rangle - \quad 2\langle \delta P_1\, \delta P_2\rangle, \\ \langle \delta R_{34}\, \delta R_{34}\rangle &= \langle \delta P_4\, \delta P_4\rangle + \langle \delta P_3\, \delta P_3\rangle - \quad 2\langle \delta P_3\, \delta P_4\rangle, \\ \langle \delta R_{12}\, \delta R_{34}\rangle &= \langle \delta P_1\, \delta P_3\rangle + \langle \delta P_2\, \delta P_4\rangle - \quad \langle \delta P_1\, \delta P_4\rangle \quad - \langle \delta P_2\, \delta P_3\rangle. \end{aligned} \tag{A-27}$$

We recognize from Eq. (A-27) that we need the complete relative covariance matrix of the P_i to be able to deduce the relative covariance matrix of the ratios. Since Table 2 contains the complete information about the uncertainty components and correlations of the P_i, the generation of this relative covariance matrix is straightforward, as shown in Table 3. With the result of Table 3 we can determine the relative covariance matrix (in %^{2}) of the measured ratios shown in Eq. (A-27) as

$$\begin{pmatrix} \langle \delta R_{12}\, \delta R_{12}\rangle & \langle \delta R_{12}\, \delta R_{34}\rangle \\ \langle \delta R_{34}\, \delta R_{12}\rangle & \langle \delta R_{34}\, \delta R_{34}\rangle \end{pmatrix} = \begin{pmatrix} 13.72 & -1.14 \\ -1.14 & 17.87 \end{pmatrix}. \tag{A-28}$$

The final result is then given by:

Ratio				Rel.Std. Dev. %	Correlation Matrix(× 100)
$\sigma_2\left[^{27}\mathrm{Al(n,p)}\right]$ / $\sigma_1\left[^{27}\mathrm{Al(n,}\alpha\mathrm{)}\right]$	=	4.797		3.70	$\begin{pmatrix} 100 & \\ \boxed{\text{A3-2}} & 100 \end{pmatrix}$.
$\sigma_4\left[^{24}\mathrm{Mg(n,p)}\right]$ / $\sigma_3\left[^{115}\mathrm{In(n,n')}\right]$	=	0.009651	$\boxed{\text{A3-1}}$		

Table 3: Combination of the Various Uncertainty Components

$$
\begin{array}{c} \\ i=1 \\ 2 \\ 3 \\ 4 \\ j= \end{array}
\begin{array}{c} \langle \delta A_i\ \delta A_j \rangle \\ \left(\begin{array}{cccc} 1.6^2 & & & \\ 0 & 2.0^2 & & \\ 0 & 0 & 1.0^2 & \\ 0 & 0 & 0 & 3.2^2 \end{array} \right) \\ \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \end{array}
+
\begin{array}{c} \langle \delta \epsilon_i\ \delta \epsilon_j \rangle \\ \left(\begin{array}{cccc} \boxed{\text{A3-3}}^2 & & & \\ \boxed{\text{A3-4}} \times 1.1 \times 1.4 & \boxed{\text{A3-5}}^2 & & \\ \boxed{\text{A3-6}} \times 1.1 \times 2.2 & 0.95 \times \boxed{\text{A3-7}} \times 2.2 & \boxed{\text{A3-8}}^2 & \\ \boxed{\text{A3-9}} \times 1.1 \times 1.1 & 0.94 \times \boxed{\text{A3-10}} \times 1.1 & 0.80 \times 2.2 \times 1.1 & \boxed{\text{A3-11}}^2 \end{array} \right) \end{array}
$$

$$
+
\begin{array}{c} \langle \delta k_i^G\ \delta k_j^G \rangle \\ \left(\begin{array}{cccc} \boxed{\text{A3-12}}^2 & & & \\ \boxed{\text{A3-13}}^2 & \boxed{\text{A3-14}}^2 & & \\ \boxed{\text{A3-15}}^2 & \boxed{\text{A3-16}}^2 & \boxed{\text{A3-17}}^2 & \\ \boxed{\text{A3-18}}^2 & \boxed{\text{A3-19}}^2 & \boxed{\text{A3-20}}^2 & \boxed{\text{A3-21}}^2 \end{array} \right) \end{array}
+
\begin{array}{c} \langle \delta k_i^T\ \delta k_j^T \rangle \\ \left(\begin{array}{cccc} 0.2^2 & & & \\ 0 & 0 & & \\ 0 & 0 & 0 & \\ 0.2^2 & 0 & 0 & 0.2^2 \end{array} \right) \end{array}
+
\begin{array}{c} \langle \delta N_i\ \delta N_j \rangle \\ \left(\begin{array}{cccc} \boxed{\text{A3-22}}^2 & & & \\ \boxed{\text{A3-23}}^2 & \boxed{\text{A3-24}}^2 & & \\ \boxed{\text{A3-25}}^2 & \boxed{\text{A3-26}}^2 & \boxed{\text{A3-27}}^2 & \\ \boxed{\text{A3-28}}^2 & \boxed{\text{A3-29}}^2 & \boxed{\text{A3-30}}^2 & \boxed{\text{A3-31}}^2 \end{array} \right) \end{array}
$$

$$
+
\begin{array}{c} \langle \delta k_i^B\ \delta k_j^B \rangle \\ \left(\begin{array}{cccc} 0.7^2 & & & \\ 0.7 \times 1.0 & 1.0^2 & & \\ 0.7 \times 1.0 & 1.0 \times 1.0 & 1.0^2 & \\ 0.7 \times 0.7 & 1.0 \times 0.7 & 1.0 \times 0.7 & 0.7^2 \end{array} \right) \end{array}
+
\begin{array}{c} \langle \delta k_i^H\ \delta k_j^H \rangle \\ \left(\begin{array}{cccc} \boxed{\text{A3-32}}^2 & & & \\ \boxed{\text{A3-33}}^2 & \boxed{\text{A3-34}}^2 & & \\ \boxed{\text{A3-35}}^2 & \boxed{\text{A3-36}}^2 & \boxed{\text{A3-37}}^2 & \\ \boxed{\text{A3-38}}^2 & \boxed{\text{A3-39}}^2 & \boxed{\text{A3-40}}^2 & \boxed{\text{A3-41}}^2 \end{array} \right) \end{array}
$$

$$
+
\begin{array}{c} \langle \delta k_i^S\ \delta k_j^S \rangle \\ \left(\begin{array}{cccc} 0.5^2 & & & \\ 0 & 0.5^2 & & \\ 0 & 0 & 1.0^2 & \\ 0.5^2 & 0 & 0 & 0.5^2 \end{array} \right) \end{array}
+
\begin{array}{c} \langle \delta k_i^J\ \delta k_j^J \rangle \\ \left(\begin{array}{cccc} 0.1^2 & & & \\ 0 & 1.0^2 & & \\ 0 & 0 & 1.0^2 & \\ 0.1^2 & 0 & 0 & 0.1^2 \end{array} \right) \end{array}
+
\begin{array}{c} \langle \delta k_i^R\ \delta k_j^R \rangle \\ \left(\begin{array}{cccc} 1.0^2 & & & \\ 0 & 1.0^2 & & \\ 0 & 0 & 1.0^2 & \\ 0 & 0 & 0 & 1.0^2 \end{array} \right) \end{array}
$$

$$
=
\begin{array}{c} \langle \delta P_i\ \delta P_j \rangle \\ \left(\begin{array}{cccc} 9.58 & & & \\ 6.16 & 16.46 & & \\ 6.64 & 7.93 & 13.86 & \\ 6.00 & 6.15 & 6.64 & 17.29 \end{array} \right) \end{array}
$$

2 Weighted Average and Least-Squares

2.1 Basic Formulae

- For two quantities y_1 and y_2 related by the covariance matrix $\boldsymbol{V}$, the off-diagonal weighted average p and its variance $(\Delta p)^2$ are
  - $p = \dfrac{(V_{22} - V_{12})y_1 + (V_{11} - V_{12})y_2}{V_{11} + V_{22} - 2V_{12}}$
  - $(\Delta p)^2 = \dfrac{V_{11}V_{22} - V_{12}^2}{V_{11} + V_{22} - 2V_{12}}$
- If parameters $\boldsymbol{p_0}$ (covariance $\boldsymbol{M_0}$) for modelling (fitting) function $\boldsymbol{y} \sim \boldsymbol{f}(\boldsymbol{p})$ are updated by experimental data points $\boldsymbol{y}$ (covariance $\boldsymbol{V}$), updated fitting parameters $\boldsymbol{p}$ and its covariance $\boldsymbol{M}$ are
  - $\boldsymbol{p} = \boldsymbol{p_0} + \boldsymbol{M_0}\boldsymbol{G}^t(\boldsymbol{G}\boldsymbol{M_0}\boldsymbol{G}^t + \boldsymbol{V})^{-1}(\boldsymbol{y} - \boldsymbol{y_0})$,
  - $\boldsymbol{M} = \boldsymbol{M_0} - \boldsymbol{M_0}\boldsymbol{G}^t(\boldsymbol{G}\boldsymbol{M_0}\boldsymbol{G}^t + \boldsymbol{V})^{-1}\boldsymbol{G}\boldsymbol{M_0}$,

  where $\boldsymbol{y_0}=\boldsymbol{f}(\boldsymbol{p_0})$ and $\boldsymbol{G}$ is $\partial \boldsymbol{f}/\partial \boldsymbol{p}|_{\boldsymbol{p}=\boldsymbol{p_0}}$.

2.2 Peelle's Pertinent Puzzle

Two experimental data points $y_1 = 1.5$ and $y_2 = 1.0$ were obtained for a physical quantity. They were derived from count rates A_1 and A_2 and a common normalization factor N by $y_1 = NA_1$ and $y_2 = NA_2$. The fractional uncertainty $\Delta A_1/A_1 = \Delta A_2/A_2 = 10\%$, while the fractional uncertainty $\Delta N/N = 20\%$.

If we treat both the count rate and normalization factor as uncorrelated between two measurements, the fractional covariance matrix between y_1 and y_2 becomes

$$\boldsymbol{v} = \begin{pmatrix} \boxed{\text{B1-1}} & \\ 0.00 & \boxed{\text{B1-2}} \end{pmatrix}, \tag{B-1}$$

and the corresponding covariance matrix is

$$\boldsymbol{V} = \begin{pmatrix} \boxed{\text{B1-3}} & \\ 0.0000 & \boxed{\text{B1-4}} \end{pmatrix}. \tag{B-2}$$

Therefore the weighted-average becomes $p =$ B1-5 and its standard deviation is $\Delta p=$ B1-6.

If we treat the count rate as uncorrelated while the normalization factor as fully correlated,

$$\boldsymbol{v} = \begin{pmatrix} 0.05 & \\ \boxed{\text{B1-7}} & \boxed{\text{B1-8}} \end{pmatrix}, \tag{B-3}$$

and the corresponding covariance matrix is

$$\boldsymbol{V} = \begin{pmatrix} 0.1125 & \\ \boxed{\text{B1-9}} & \boxed{\text{B1-10}} \end{pmatrix}. \tag{B-4}$$

Therefore the weighted-average becomes $p =$ B1-11 and its standard deviation is $\Delta p=$ B1-12. Namely the weighted-average becomes lower than both experimental data points if we consider the correlation property of the normalization factor - Peelle's Pertinent Puzzle (PPP) found by Robert Peelle (ORNL) in 1987 [4].

2.3 Evaluation of Spectrum-Averaged Cross Sections [*4]

We assume that two independent experiments exist (performed by different experimenters) of cross sections averaged over a Cf-252 neutron spectrum. Our aim is to combine both these data sets to obtain the most consistent "best" set of data. The first experiment comprises the data of two reactions:

Table 4: Experiment No. 1

Neutron Reaction	Spectrum-Averaged Cross Section	Rel.Std.Dev. %	Correlation Matrix (× 100)	
^{235}U(n,f)	1215 mb	1.79	100	
^{239}Pu(n,f)	1790 mb	2.26	59	100

In the second experiment the cross section of the reaction ^{235}U(n,f) is measured twice (using a slightly different method in the second case), and, instead of the absolute cross section of ^{239}Pu(n,f) a ratio measurement relative to ^{235}U(n,f) was performed.

Table 5: Experiment No. 2

Neutron Reaction (Ratio)	Spectrum-Averaged Cross Section (Ratio)	Rel.Std.Dev. %	Correlation Matrix (× 100)		
^{235}U(n,f)	1205 mb	2.25	100		
^{235}U(n,f)	1203 mb	3.02	80	100	
^{239}Pu(n,f)/^{235}U(n,f)	1.500	1.33	−19	−5	100

A first glance at Table 5, makes one astonished why an average value of the first and second measurement was not taken. In principle it is not difficult to calculate such an average (also with regard to existing covariances). However, an average can only be formed if no further correlations to any other data exist of the data contributing to the average. If we look at Table 5 we recognize correlations between the first as well as the second data and the third data. In such a case the average would ignore the existing correlation to the third data. This means that an average, which is (as will be shown later) equivalent with the least squares procedure, cannot be calculated for a subset of the total data contributing to the least squares.

Thus the given example demonstrates two important aspects of the data evaluation process:

a) the combination of data of the same type which have been determined more than once

b) the connection between absolute and relative cross section data.

In our example we regard the data of the first experiment (Table 4) as an initial estimates of the final data $\boldsymbol{p_0}$, i,e.:

$$\boldsymbol{p_0} = \begin{pmatrix} \sigma_1 = 1215 \\ \sigma_2 = 1790 \end{pmatrix} \quad \text{and} \quad \boldsymbol{M_0} = \begin{pmatrix} 473.0 & \\ \boxed{\text{B3-1}} & \boxed{\text{B3-2}} \end{pmatrix}, \tag{B-5}$$

[*4] Extraction from Ref. [1] with minor modification.

and the data of the second experiment (Table 5) as "experimental data $\boldsymbol{y}$":

$$\boldsymbol{y} = \begin{pmatrix} 1205 \\ 1203 \\ 1.500 \end{pmatrix} \quad \text{with} \quad \boldsymbol{V} = \begin{pmatrix} 7.351\text{E}+2 & & \\ \boxed{\text{B3-3}} & \boxed{\text{B3-4}} & \\ \boxed{\text{B3-5}} & \boxed{\text{B3-6}} & \boxed{\text{B3-7}} \end{pmatrix} \tag{B-6}$$

The vector $\boldsymbol{y_0}$ which represents the fit function at the parameter estimates $\boldsymbol{p_0}$ is then:

$$\boldsymbol{y_0} = \begin{pmatrix} \sigma_1 = 1215 \\ \sigma_1 = 1215 \\ \sigma_2/\sigma_1 = 1.473 \end{pmatrix}, \tag{B-7}$$

and the G matrix is given by:

$$\boldsymbol{G} = \begin{pmatrix} \partial\sigma_1/\partial\sigma_1 & \partial\sigma_1/\partial\sigma_2 \\ \partial\sigma_1/\partial\sigma_1 & \partial\sigma_1/\partial\sigma_2 \\ \partial(\sigma_2/\sigma_1)/\partial\sigma_1 & \partial(\sigma_2/\sigma_1)/\partial\sigma_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ -\sigma_2/\sigma_1^2 & 1/\sigma_1 \end{pmatrix}. \tag{B-8}$$

The first column of Eq. (B-8) corresponds to the first parameter, σ_1, and the second column to the second parameter, σ_2, while the rows correspond to the data 1 to 3. The data no. 1 and no. 2 are identical (within their uncertainties) with the first parameter, so we have unity as both first elements of the first column and a corresponding zero in the second column. Data no. 3 (the ratio measurement) depends on both parameters which is expressed in the corresponding derivatives in row 3, columns 1 and 2.

Inserting the results of Eq. (B-5) - (B-8) in the least squares formalism, we obtain as a final result:

$$\boldsymbol{p} = \begin{pmatrix} 1210 \\ 1805 \end{pmatrix} \quad \text{and} \quad \boldsymbol{M} = \begin{pmatrix} 285.0 & \\ 349.0 & 789.9 \end{pmatrix} \tag{B-9}$$

Table 6: Evaluated Data

Neutron Reaction	Spectrum-Averaged Cross Section	Rel.Std.Dev. %	Correlation Matrix (× 100)	
^{235}U(n,f)	B3-8 mb	B3-10	B3-12	
^{239}Pu(n,f)	B3-9 mb	B3-11	B3-13	B3-14

2.4 Carbon Resonance Energy by Two TOF Measurement Data [5]

The energy of the 2080 keV carbon resonance was measured at Harwell by James [6]. The neutron resonance energy E_i (eV) obtained by the i-th run ($i = 1, 2$) is related with the flight path length L_i (m) and time-of-flight t_i (μsec) by

$$E_i(L_i, t_i) = (72.3 L_i/t_i)^2. \tag{B-10}$$

Two flight path lengths (L_1 and L_2) are considered as independent, while time-of-flight (t_1 and t_2) are decomposed to the uncorrelated part (t_{c1} and t_{c2}) and fully correlated part (t_m) as $t_1 = t_m + t_{c1}$ and $t_2 = t_m + t_{c2}$. The experimental data from the measurement are summarized in Table 7. According to the error propagation

Table 7:

Exp.No.	L_i(m)	ΔL_i(m)	Δt_m(μsec)	Δt_{ci}(μsec)	E_i (eV)
1	100	0.003	0.40×10^{-3}	0.25×10^{-3}	2078.31×10^{3}
2	50	0.006	0.40×10^{-3}	0.50×10^{-3}	2079.20×10^{3}

formula for general functions, the covariance between E_i and E_j ($i, j = 1, 2$) is given by

$$V_{11} = (\partial E_1/\partial L_1)^2 (\Delta L_1)^2 + (\partial E_1/\partial t_1)^2 (\Delta t_1)^2, \tag{B-11}$$
$$V_{22} = (\partial E_2/\partial L_2)^2 (\Delta L_2)^2 + (\partial E_2/\partial t_2)^2 (\Delta t_2)^2, \tag{B-12}$$
$$V_{12} = (\partial E_1/\partial t_1)(\partial E_2/\partial t_2) V_{t_1 t_2}. \tag{B-13}$$

Note that all terms involving correlation between the flight path length (L) and time-of-flight (t) become zero. These partial derivatives can be calculated by using Eq. (B-10), and we obtain the following covariances:

$$v_{11} = \boxed{\text{B2-1}}(f_{L_1}^2 + f_{t_1}^2), \tag{B-14}$$
$$v_{22} = \boxed{\text{B2-2}}(f_{L_2}^2 + f_{t_2}^2), \tag{B-15}$$
$$v_{12} = \boxed{\text{B2-3}} v_{t_1 t_2}, \tag{B-16}$$

where $f_{L_i}^2 = (\Delta L_i/L_i)^2$, $f_{t_i}^2 = (\Delta t_i/t_i)^2 = (\Delta t_i)^2 E_i/(72.3 L_i)^2$, $v_{t_1 t_2} = V_{t_1 t_2}/(t_1 t_2) = V_{t_1 t_2}\sqrt{E_1 E_2}/(72.3^2 L_1 L_2)$.

Two time-of-flight t_1 and t_2 are linear combinations of t_m, t_{c1} and t_{c2}. Following the error propagation formula for linear combination, the covariance $V_{t_1 t_1} = (\Delta t_1)^2$, $V_{t_2 t_2} = (\Delta t_2)^2$ and $V_{t_1 t_2}$ are

$$V_{t_1 t_1} = V_{t_m t_m} + V_{t_{c1} t_{c1}} = (\Delta t_m)^2 + (\Delta t_{c1})^2, \tag{B-17}$$
$$V_{t_2 t_2} = V_{t_m t_m} + V_{t_{c2} t_{c2}} = (\Delta t_m)^2 + (\Delta t_{c2})^2, \tag{B-18}$$
$$V_{t_1 t_2} = V_{t_m t_m} = (\Delta t_m)^2. \tag{B-19}$$

From these equations and Table 7, we can calculate the fractional variances of the resonance energies $\boldsymbol{v} = \boldsymbol{V}/(E_1 E_2)$:

$$\boldsymbol{v} = \begin{pmatrix} 3.90\times10^{-8} & \\ \boxed{\text{B2-4}} & \boxed{\text{B2-5}} \end{pmatrix}, \tag{B-20}$$

which corresponds to

$$\boldsymbol{V} = \begin{pmatrix} 0.168 & \\ \boxed{\text{B2-6}} & \boxed{\text{B2-7}} \end{pmatrix} \text{keV}^2. \tag{B-21}$$

The off-diagonal weighted average of two resonance energies $E =$ $\boxed{\text{B2-8}}$ keV, and its standard deviation $\Delta E =$ $\boxed{\text{B2-9}}$ keV. This average is lower than both E_1 and E_2.

3 Usage of SOK (Simultaneous Evaluation on KALMAN) [*5]

The SOK code requires :

1. experimental data (UNIT 10), data error (UNIT 11), and correlation matrices (UNIT 12)
2. prior parameters (UNIT 50) and their uncertainties (UNIT 51)
3. control data (UNIT 5)

where the UNIT *N* is the FORTRAN logical unit number for I/O. The correlation file (UNIT 12) is optional.

In this section, a data file allocated to UNIT *N* is called as "fort.*n*".

3.1 Description of Experimental Data

An experimental database is separated into three files — cross section data (E_n, σ), their uncertainties (E_n, $\Delta\sigma$), and their correlation matrix. These three files are allocated to the FORTRAN logical UNITs of 10, 11, and 12, respectively.

One measurement contains several data points. These cross section data and their errors are stored with the following formats:

Cross section Data File – fort.10

```
(A43,I5)    TITLE, ND
(6E11.4)    (X(I),Y(I),I=1,ND)
```

Data Error File – fort.11

```
(43X,I5)    ND
(6E11.4)    (DUMMY,Z(I),I=1,ND)
```

where `TITLE` is an arbitrary text, `ND` is the number of energy points, `X`, `Y`, and `Z` are the energy, cross section, and its uncertainty. The units of energies and cross sections are arbitrary, but the same units must be used for all experimental data. If `Z` is positive, the uncertainty `Z` is a relative error. If `Z` is negative, this value is interpreted as an absolute error. For example, `0.03` is 3%, and `Z=-0.1` represents ± `0.1`.

A correlation matrix of the experimental data is read from UNIT 12.

Correlation File – fort.12

```
(43X,I5)     NC
             DO I=1,NC
(12F6.3)        (V(I*(I-1)/2+J),J=1,I)
```

where `V` is the correlation ($-1 \leq$ `V` ≤ 1), and `NC` is the number of energy points. Usually `NC` must be the same as `ND`, but one can omit the correlation data by setting `NC=0`.

A set of data describes one measurement of a reaction type. When there are several measurements of various reaction types, those data are stored sequentially in fort.10, 11, and 12. The order of experimental

[*5] Extraction from Ref. [7] with minor modification.

data is arbitrary, but the same order should be used for the data, error, and correlation files. The order of experimental data is defined in the control data given in UNIT 5. When there are six experimental data sets (three measurements of reaction *A*, two of reaction *B*, and one of *C*), the structure of the experimental data files becomes as follows.

Data number 1 of Reaction *A*
Data number 2 of Reaction *A*
Data number 3 of Reaction *A*
Data number 1 of Reaction *B*
Data number 2 of Reaction *B*
Data number 1 of Reaction *C*

The followings are examples of the data files which contain three measurements.

```
    ----*----1----*----2----*----3----*----4----*----5----*----6----*----7
 1: Data 1                                            5
 2:  1.4700E+01 6.7300E-01 1.6000E+01 4.5100E-01 1.7000E+01 3.6600E-01
 3:  1.8000E+01 2.3400E-01 1.9000E+01 2.7300E-01
 4: Data 2                                           14
 5:  6.4200E+00 6.0000E-02 6.8000E+00 2.7000E-01 6.9600E+00 5.4000E-01
 6:  7.0000E+00 4.7000E-01 7.2000E+00 5.1000E-01 7.2500E+00 7.9000E-01
 7:  7.4500E+00 8.9000E-01 7.5800E+00 9.8000E-01 7.8200E+00 1.1100E+00
 8:  7.8800E+00 1.0700E+00 8.4900E+00 1.2100E+00 8.9600E+00 1.3900E+00
 9:  9.4800E+00 1.4600E+00 9.9700E+00 1.4900E+00
10: Data 3                                           10
11:  6.8900E+00 2.3300E-01 7.4100E+00 6.0400E-01 7.6700E+00 8.1100E-01
12:  7.9300E+00 8.7900E-01 8.1800E+00 9.9900E-01 8.4400E+00 1.0720E+00
13:  8.6900E+00 1.0290E+00 8.9400E+00 1.1560E+00 9.4400E+00 1.1710E+00
14:  9.9300E+00 1.2320E+00

    ----*----1----*----2----*----3----*----4----*----5----*----6----*----7
 1: Error 1                                           5
 2:  1.4700E+01 6.1000E-02 1.6000E+01 1.8000E-01 1.7000E+01 2.0000E-01
 3:  1.8000E+01 3.6000E-01 1.9000E+01 3.2000E-01
 4: Error 2                                          14
 5:  6.4200E+00 3.0000E-02 6.8000E+00 2.0000E-02 6.9600E+00 4.0000E-02
 6:  7.0000E+00 3.0000E-02 7.2000E+00 4.0000E-02 7.2500E+00 5.0000E-02
 7:  7.4500E+00 5.0000E-02 7.5800E+00 5.0000E-02 7.8200E+00 5.0000E-02
 8:  7.8800E+00 5.0000E-02 8.4900E+00 5.0000E-02 8.9600E+00 5.0000E-02
 9:  9.4800E+00 5.0000E-02 9.9700E+00 5.0000E-02
10: Error 3                                          10
11:  6.8900E+00-3.9000E-02 7.4100E+00-5.4000E-02 7.6700E+00-6.2000E-02
12:  7.9300E+00-4.8000E-02 8.1800E+00-4.1000E-02 8.4400E+00-5.2000E-02
13:  8.6900E+00-6.0000E-02 8.9400E+00-4.2000E-02 9.4400E+00-4.6000E-02
14:  9.9300E+00-4.4000E-02
```

```
    ----*----1----*----2----*----3----*----4----*----5----*----6----*----7
 1: Correlation 1                                    5
 2:  1.000
 3:  0.111 1.000
 4:  0.098 0.033 1.000
 5:  0.055 0.019 0.016 1.000
 6:  0.062 0.022 0.019 0.010 1.000
 7: Correlation 2                                    0
 8: Correlation 3                                   10
 9:  1.000
10:  0.060 1.000
11:  0.070 0.132 1.000
12:  0.098 0.184 0.216 1.000
13:  0.131 0.245 0.287 0.402 1.000
14:  0.111 0.208 0.243 0.340 0.452 1.000
15:  0.092 0.173 0.202 0.283 0.376 0.318 1.000
16:  0.148 0.277 0.324 0.454 0.604 0.511 0.425 1.000
17:  0.137 0.256 0.300 0.420 0.558 0.472 0.393 0.631 1.000
18:  0.151 0.282 0.330 0.461 0.614 0.520 0.432 0.694 0.642 1.000
```

3.2 Description of Prior Parameters

The SOK code reads prior cross sections and their uncertainties from UNIT 50 and 51.

Prior Cross Section File – fort.50

```
(A43,I5)   TITLE, NE
(6E11.4)   (E0(I),P0(I),I=1,NE)
```

Prior Cross Section Error File – fort.51

```
(A43,I5)   TITLE, NE
(6E11.4)   (DUMMY,PE(I),I=1,NE)
```

where `TITLE` is an arbitrary text, `NE` is the number of energy points, `E0` and `P0` are an energy and a cross section, and `PE` is a prior uncertainty. The uncertainties are relative errors. The units of energies and cross sections must be the same as those of the experimental data read from UNITs 10 and 11.

Currently there is no way to give a prior covariance of the cross section. The uncertainties of the prior cross sections are regarded as uncorrelated.

The above data describe one type of cross sections. When several cross sections are evaluated simultaneously, these data are concatenated and stored in fort.50 and 51. One can use different energy points for each cross section type. The number of cross sections is calculated automatically, and it is referred to as `NKIND` in the code. The order of the cross sections in these files is used to specify the reaction type. These numbers (from 1 to `NKIND`) are an index of each reaction. The maximal number of `NKIND` is 99.

The following examples present the data files which contain two cross section types (`NKIND=2`). The prior uncertainties assumed are 50% for all.

```
    ----*----1----*----2----*----3----*----4----*----5----*----6----*----7
 1: Inelastic 1st level                                  24
 2:  1.0000E-02 6.5979E+00 1.0000E-01 2.7476E+00 5.0000E-01 1.9889E+00
 3:  7.5000E-01 1.6267E+00 1.0000E+00 1.4527E+00 1.2500E+00 1.3435E+00
 4:  1.5000E+00 1.2662E+00 1.7500E+00 1.2078E+00 2.0000E+00 1.1615E+00
 5:  2.2500E+00 1.0919E+00 2.5000E+00 1.0162E+00 3.0000E+00 8.3853E-01
 6:  4.0000E+00 5.9353E-01 5.0000E+00 4.1736E-01 6.0000E+00 3.2365E-01
 7:  8.0000E+00 1.7176E-01 1.0000E+01 1.0063E-01 1.2000E+01 3.4596E-02
 8:  1.3000E+01 2.4942E-02 1.4000E+01 1.7562E-02 1.5000E+01 1.2131E-02
 9:  1.6000E+01 8.2704E-03 1.8000E+01 3.7694E-03 2.0000E+01 1.7137E-03
10: Inelastic 2nd level                                  24
11:  1.0000E-02 0.0000E+00 1.0000E-01 0.0000E+00 5.0000E-01 1.3546E-01
12:  7.5000E-01 3.6810E-01 1.0000E+00 4.4806E-01 1.2500E+00 4.8766E-01
13:  1.5000E+00 5.1221E-01 1.7500E+00 5.2979E-01 2.0000E+00 5.4338E-01
14:  2.2500E+00 5.3302E-01 2.5000E+00 5.1264E-01 3.0000E+00 4.5885E-01
15:  4.0000E+00 3.5950E-01 5.0000E+00 2.7149E-01 6.0000E+00 2.2053E-01
16:  8.0000E+00 1.2464E-01 1.0000E+01 7.5152E-02 1.2000E+01 4.3703E-02
17:  1.3000E+01 3.1578E-02 1.4000E+01 2.2305E-02 1.5000E+01 1.5467E-02
18:  1.6000E+01 1.0586E-02 1.8000E+01 4.8735E-03 2.0000E+01 2.2361E-03

    ----*----1----*----2----*----3----*----4----*----5----*----6----*----7
 1: Inelastic 1st level                                  24
 2:  1.0000E-02 5.0000E-01 1.0000E-01 5.0000E-01 5.0000E-01 5.0000E-01
 3:  7.5000E-01 5.0000E-01 1.0000E+00 5.0000E-01 1.2500E+00 5.0000E-01
 4:  1.5000E+00 5.0000E-01 1.7500E+00 5.0000E-01 2.0000E+00 5.0000E-01
 5:  2.2500E+00 5.0000E-01 2.5000E+00 5.0000E-01 3.0000E+00 5.0000E-01
 6:  4.0000E+00 5.0000E-01 5.0000E+00 5.0000E-01 6.0000E+00 5.0000E-01
 7:  8.0000E+00 5.0000E-01 1.0000E+01 5.0000E-01 1.2000E+01 5.0000E-01
 8:  1.3000E+01 5.0000E-01 1.4000E+01 5.0000E-01 1.5000E+01 5.0000E-01
 9:  1.6000E+01 5.0000E-01 1.8000E+01 5.0000E-01 2.0000E+01 5.0000E-01
10: Inelastic 2nd level                                  24
11:  1.0000E-02 5.0000E-01 1.0000E-01 5.0000E-01 5.0000E-01 5.0000E-01
12:  7.5000E-01 5.0000E-01 1.0000E+00 5.0000E-01 1.2500E+00 5.0000E-01
13:  1.5000E+00 5.0000E-01 1.7500E+00 5.0000E-01 2.0000E+00 5.0000E-01
14:  2.2500E+00 5.0000E-01 2.5000E+00 5.0000E-01 3.0000E+00 5.0000E-01
15:  4.0000E+00 5.0000E-01 5.0000E+00 5.0000E-01 6.0000E+00 5.0000E-01
16:  8.0000E+00 5.0000E-01 1.0000E+01 5.0000E-01 1.2000E+01 5.0000E-01
17:  1.3000E+01 5.0000E-01 1.4000E+01 5.0000E-01 1.5000E+01 5.0000E-01
18:  1.6000E+01 5.0000E-01 1.8000E+01 5.0000E-01 2.0000E+01 5.0000E-01
```

3.3 Description of Input Data

The input data controls the calculational flow and the sequence of the experimental data in fort.10, 11, and 12. Since the experimental database contains several measurements with the different reaction types, the database is divided into several blocks with the same reaction. The sequence of the blocks and the order of the measurements within the block are defined in this input file.

```
(A80)       TITLE
(4I5)       NREAC,KCOVEX,KCTL1,KCTL2
            DO I=1,NREAC
(14I5)         IEXP(I),NMSUR
(7E10.3)       (EW(J),J=1,NMSUR)
```

where TITLE is the title of the calculation, NREAC is the number of blocks in the experimental database. The index IEXP tells a type of reaction and NMSUR is the number of measurements in the block.

When the experimental database has the following structure, this database is divided into three blocks — reaction types *A*, *B*, and *C* — then NREAC=3. Each block contains four, three, and two measurements, then NMSUR=4 for the reaction type *A*, NMSUR=3 for *B*, and NMSUR=2 for *C*.

Data number 1 of Reaction *A*
Data number 2 of Reaction *A*
Data number 3 of Reaction *A*
Data number 4 of Reaction *A*
Data number 1 of Reaction *B*
Data number 2 of Reaction *B*
Data number 3 of Reaction *B*
Data number 1 of Reaction *C*
Data number 2 of Reaction *C*

An integer number called an index is used to identify the reaction type. The index is the order of the cross sections in fort.50 and 51. The first cross section in those files has the index of "1", and the second one is "2", and so on. If the experimental data is a ratio measurement which corresponds to a ratio of the index a to b, this index is given as $100 \times a + b$.

Let us consider an example. In the case of evaluation of ^{235}U and ^{238}U fission cross sections, fort.50 and 51 contain their prior values in this order. The index for ^{235}U is 1, while ^{238}U is 2, then NKIND becomes 2. If the experimental database (fort.10, 11, and 12) contains one measurement which is a fission cross section ratio of ^{238}U to ^{235}U, the index of the measurement IEXP becomes 201, and the number of reaction block becomes NREAC=1.

One can manipulate a weight of each measurement by EW. The uncertainties of the corresponding experimental data are multiplied by the value of EW. If EW=0, the measurement is ignored. Usually EW is unity.

KCOVEX, KCTL1, and KCTL2 are the flags. If KCOVEX=0, the SOK code does not read correlation data, otherwise it reads correlation data from UNIT 12. A χ^2 test can be done with the flag KCTL1. The SOK code calculates the χ^2 value when KCTL1=N. The cross sections and their uncertainties are read from UNIT N and $N+1$ with the same format as the data in fort.50 and 51. Therefore, if KCTL1=50, it gives the χ^2 value for the prior cross sections. If KCTL2=1, smoothly interpolated posterior cross sections are generated by means of the cubic-spline interpolation.

An example of the input data is as follows:

```
    ----*----1----*----2----*----3----*----4----*----5----*----6----*----7
 1: SOK INPUT DATA
 2:     3    1    0    1
 3:     1    4
 4:  1.000E+00 1.000E+00 1.000E+00 1.000E+00
 5:     2    3
 6:  1.000E+00 0.0       1.000E+00
 7:   102    2
 8:  1.000E+00 1.000E+00
```

The number of measurements is 9 (= 4 + 3 + 2), and there are three blocks (NREAC=3). The first block is a type "1", and there are four measurements. The next block is a type "2". Three measurements are stored in the file, but the second measurement is ignored. The last block contains two measurements, those are the ratios of the cross sections "1" to "2".

3.4 Output

The SOK code prints χ^2 values and the number of data points for each measurement during execution, and finally it prints the posterior cross sections and their uncertainties. The following is an example of the output.

```
      ----*----1----*----2----*----3----*----4----*----5----*----6----*----7
    1: Simultaneous Evaluation for JENDL-3.3
    2: NUMBER OF DATA BLOCKS      6
    3: NUMBER OF SPLINE KNOTS   211
    4:
    5: # 21463002 P.H.White                    1965    6
    6: *** EXP. DATA IGNORED ********
    7: CROSS SECTION :U233FIS
    8: SQ.NO.:    1   REACT.:    1   POINTS:    0   SUM UP:    0
    9: PARTIAL CHI SQ: 0.00000E+00   CUMULATIVE : 0.00000E+00
   10:
   11: # 21195002 P.H.White                    1967    4
   12: CROSS SECTION :U233FIS
   13: SQ.NO.:    2   REACT.:    2   POINTS:    4   SUM UP:    4
   14: PARTIAL CHI SQ: 9.14181E-06   CUMULATIVE : 9.14181E-06
       ...
  812: 10563002       Behrens                        107
  813: CROSS SECTION :PU241FIS    U235FIS
  814: SQ.NO.:  162   REACT.:    3   POINTS:   92   SUM UP: 4661
  815: PARTIAL CHI SQ: 1.06892E+02   CUMULATIVE : 1.56656E+04
  816:
  816: CHI-SQUARE TEST !                 CHI - S =  1.56656E+04
  817: DEGREE OF FREEDOM =  4450         RATIO   =  3.52035E+00
  818:
  819:       PARAMETER    INITIAL    FINAL      ERROR
  820:
  821:     1  2.0000E-02 2.0520E+00 2.2717E+00 1.2846E+00 ( % )
  822:     2  3.0000E-02 2.0520E+00 2.0075E+00 8.5634E-01 ( % )
  823:     3  6.0000E-02 1.8110E+00 1.7804E+00 7.4145E-01 ( % )
      ...
 1030:   209  1.7500E+01 2.3819E+00 2.3451E+00 2.1581E+00 ( % )
 1031:   210  2.0000E+01 2.3000E+00 2.1893E+00 2.7890E+00 ( % )
 1032:   211  2.2000E+01 2.3000E+00 2.3086E+00 5.8164E+00 ( % )
```

The printed errors of the parameters are multiplied by the factor $\sqrt{\chi^2/(n-m)}$, but this χ^2 value is approximate. To calculate the exact χ^2 value, repeat the same calculation but KCTL1=20.

The other information is written on files.

UNIT	contents
14	covariance matrices of the evaluated cross sections
15	evaluated cross sections and their errors
17	cubic-spline interpolated cross sections (if `KCTL2=1`)
20	evaluated cross sections (the same format as fort.50)
21	evaluated cross section errors (the same format as fort.51)
60+I	experimental data of reaction block "`I`" (`I=1,NREAC`)

REFERENCES

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[3] K. Kobayashi, I. Kimura, "Fission Spectrum Averaged Cross Sections with Standard Neutron Fields", EUR 6813, Vol. II (1980), p. 1004.

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[5] F.G. Perey, "Covariance Matrices of Experimental Data", Proceedings of an International Conference on Neutron Physics and Nuclear Data for Reactors, Harwell, United Kingdom, (September 1978), 104.

[6] G.D. James, "Neutron energy standards", NBS Special Publication 493 (1977) 319.

[7] T. Kawano et al., "Evaluation of fission cross sections and covariances for ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu", JAERI-Research 2000-004 (2000).

	A1	A2	A3	B1	B2	B3
1	0.0009	0.5	4.23	0.05	4	519.1
2	0.0004	0.8	-7	0.05	4	1636.5
3	0.0029	1.0	1.1	0.1125	4	7.880E+2
4	0.058	0.5	0.94	0.0500	5.09×10^{-8}	1.320E+3
5	0.054	0.9	1.4	1.154	3.19×10^{-7}	-1.028E-1
6	0.0013	0.3	0.80	0.186	0.220	-3.624E-2
7	0.0063	2.61	1.4	0.04	1.379	3.980E-4
8	0.0025	3.14	2.2	0.05	2078.27	1210
9	0.0025	2.40	1.00	0.0600	0.41	1805
10	0.0029	1.00	0.94	0.0500		1.40
11	1.00	0.83	1.1	0.882		1.56
12	0.80	1.00	2.0	0.218		100
13	0.80	0.80	2.0			74
14	1.00	0.87	2.0			100
15	0.0013	1.00	2.0			
16			2.0			
17			2.0			
18			2.0			
19			2.0			
20			2.0			
21			2.0			
22			0.1			
23			0.1			
24			0.1			
25			0			
26			0			
27			0.1			
28			0			
29			0			
30			0			
31			0.2			
32			0.1			
33			0			
34			1.8			
35			0			
36			0			
37			0.1			
38			0			
39			0			
40			0			
41			0.1			