On the Verification and Interpretation of the Evaluated Data Covariances

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Motivation

- **CSEWG criticisizes each release of the neutron standards evaluation. In particular, the Group have expressed concerns on the ‘small’ uncertainties of the neutron standards. So, we should try to find the additional arguments to justify the results of the neutron standards evaluation**

- **Is it possible to get progress in the evaluation methodology, especially in ways to take USU into account?**

Motivation (continued)

- Results of nuclear data evaluation carried out with statistical methods are usually presented as a vector of evaluated values and corresponding covariance matrix. As a rule for the same object (cross-section, angular distribution, neutron spectrum) there is a set of evaluations performed within the framework of various physical and statistical models. For this reason, there is a necessity to compare the uncertainty information presented in the covariance matrices

- In addition, a verification of the evaluated data is possible by means of comparison of the experimental and evaluated data covariance matrices. Exceeding evaluated uncertainty over experimental one indicates error in calculations

Comparison of the covariance matrices

The covariance matrices can be compared in different ways in dependence of definition

1) **matrix C is larger than matrix B if matrix D = C - B is positive definite (D>0)**
2) **matrix C is larger than matrix B if tr(C) > tr(B), where tr(C) – trace of the matrix C; tr(C) – sum of variances of the components of the random vector in *n*-dimensional space where basis is represented by eigenvectors**
3) **matrix C is larger than matrix B if det(C) > det(B), where det(C) – determinant of the matrix A**

tr(C) and det(C) can be considered as uncertainty of the random vector (integral uncertainty)

Definition of uncertainty of the random vector (integral uncertainty)

Let's define an uncertainty Σ for a random vector $\vec{\varepsilon}$ distributed over law with probability density $\rho_{\vec{\varepsilon}}(x_1,\ldots,x_n)$ as a volume of domain D around the mathematical expectation $\vec{b}$ where a fixed portion of the distribution (for example, α) is concentrated:

$$\Sigma = \mathrm{V}(D) \tag{1}$$

$$\alpha = \mathrm{P}\,(\vec{\varepsilon} \in D) = \int\cdots\int_D \rho_{\vec{\varepsilon}}(x_1,\ldots,x_n)dx_1\ldots dx_n \tag{2}$$

The integral can be calculated explicitly only for special domains D and special distributions (like $\rho_{\vec{\varepsilon}}(x_1,\ldots,x_n) = ((2\pi)^n \det(C))^{-1/2}$ $\exp\{-\frac{1}{2}(\vec{x}-\vec{b})^t C^{-1}(\vec{x}-\vec{b})\}$, C – covariance matrix).

Choosing an integration domain

The most preferable variant – hyper ellipsoid D = $\{\vec{x} : (\vec{x} - \vec{b})^t C^{-1} (\vec{x} - \vec{b}) \leq q(\alpha)\}$:

- in this case the domain is limited by a surface of equal probability
- for given value α such the choice provides the smallest square of domain D
- allows for analytical integration for small *n*

.

Bivariate normal distribution

The integral (2) can be rewritten as

$$\alpha = \mathrm{P}\,(\vec{\varepsilon} \in D) = \iint_D \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}} \exp\left\{-\frac{Q(x_1 x_2)}{2}\right\} dx_1 dx_2 \qquad (3)$$

where

$$Q(x_1, x_2) = \frac{1}{(1-\rho^2)}\frac{x_1^2}{\sigma_1^2} - \frac{2\rho x_1 x_2}{(1-\rho^2)\sigma_1\sigma_2} + \frac{x_2^2}{(1-\rho^2)\sigma_2^2} \equiv a_{11}x_1^2 + 2a_{12}x_1x_2 + a_{22}x_2^2 \qquad (4)$$

and

$$D = \{(x_1, x_2) : Q(x_1, x_2) \le q\} \qquad (5)$$

Bivariate normal distribution (continued)

we get value for the integral (3)

$$\alpha = P\,(\vec{\varepsilon} \in D) = \iint_D \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}} \exp\left\{-\frac{Q(x_1,x_2)}{2}\right\} dx_1 dx_2$$

$$= 1\text{-}\exp(-\frac{q}{2}) \qquad (14)$$

with quadratic form $Q(x_1,x_2)$ defined in (4) as

$$D = \left\{(x_1,x_2): \frac{1}{(1-\rho^2)}\frac{x_1^2}{\sigma_1^2} - \frac{2\rho x_1 x_2}{(1-\rho^2)\sigma_1\sigma_2} + \frac{x_2^2}{(1-\rho^2)\sigma_2^2}) \le q(\alpha)\right\} \qquad (15)$$

Bivariate normal distribution (continued)

So, the uncertainty of a random vector $\vec{\varepsilon}$ distributed over bivariate normal law equals to an area $V_2(\vec{\varepsilon})$ of ellipse

$$D=\left\{(x_1,x_2):\frac{1}{(1-\rho^2)}\frac{x_1^2}{\sigma_1^2}-\frac{2\rho x_1 x_2}{(1-\rho^2)\sigma_1\sigma_2}+\frac{x_2^2}{(1-\rho^2)\sigma_2^2})\leq q(\alpha)\right\} \quad (15)$$

where a portion α of the distribution is concentrated:

$$V_2(\vec{\varepsilon})=\pi q\sigma_1\sigma_2\sqrt{1-\rho^2}=\pi q\sigma_1\sigma_2\sqrt{\det R}=\pi q\sqrt{\det C} \quad (16),$$

where R – correlation matrix, C - covariance matrix.

All the information on the shape of the ellipse and its orientation is determined by the elements of covariance matrix (see Fig.1).

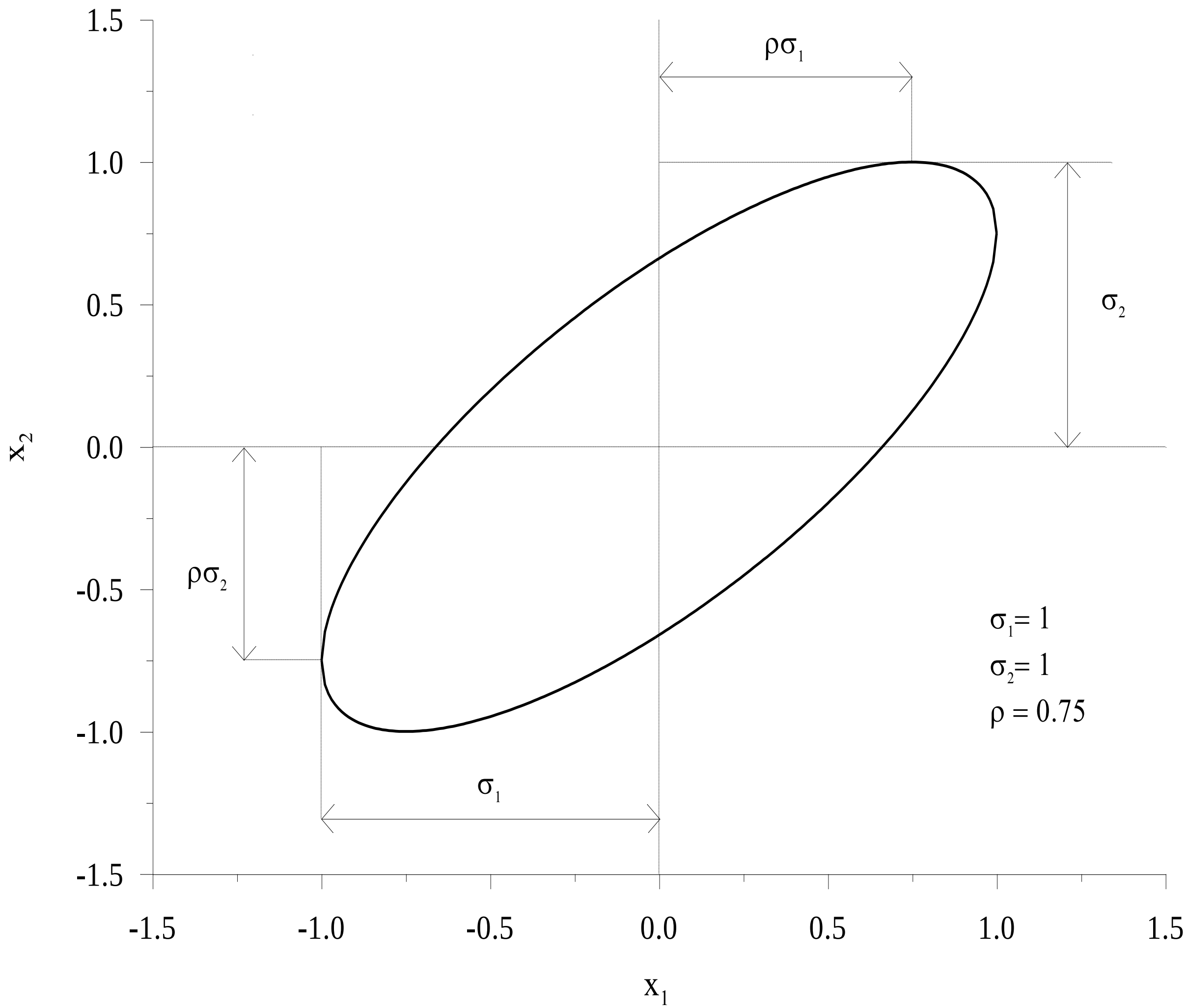


Fig.1 Scattering ellipse for a random vector distributed over bevariate normal law with zero mathematical expectation.

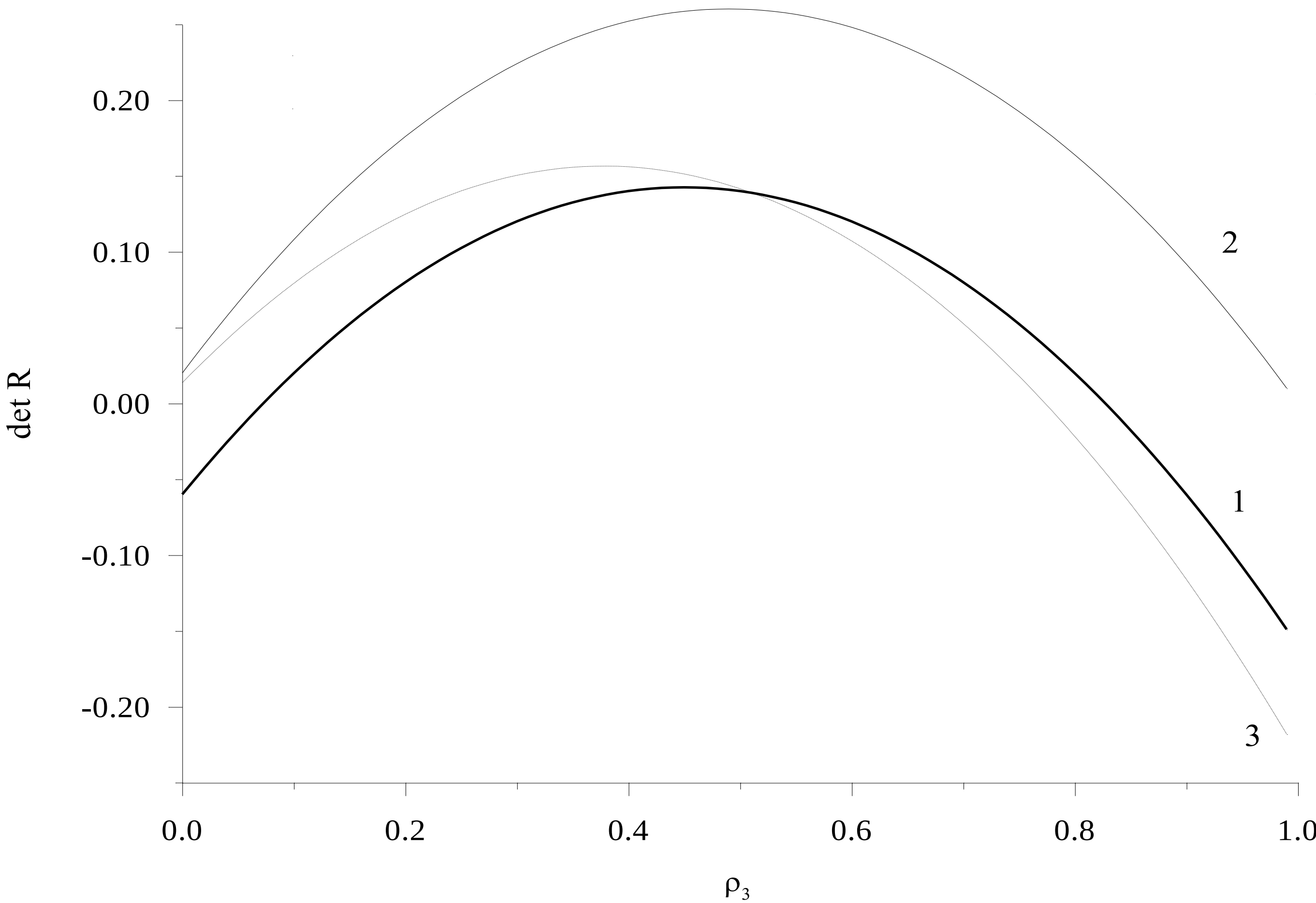
Generalization to the multidimensional random vector

For arbitrary dimension n we have a hyper ellipsoid (instead of ellipse) and the volume of hyper ellipsoid is proportional to the value $\sqrt{\det C}$ (C - covariance matrix)

$$V_n(\vec{\varepsilon}) \sim \sqrt{\det C} \tag{17}$$

For this reason the determinant of a covariance matrix can be used as a measure of uncertainty for a random vector.

Value of determinant of the correlation matrix (3x3) in dependence on correlation



Values of determinant change in a such manner that makes it possible compensation more small uncertainties of components of the random vector by more large correlations between components keeping a value of the determinant unchanged (in the range where detR>0)

Fig.2 Determinant of the correlation matrix for a random vector with 3 coordinates as function of a correlation coefficient (at fixed two other ones: curve 1 - ρ_1=0.5, ρ_2=0.9, curve 2 - ρ_1=0.7, ρ_2=0.7, curve 3 - ρ_1=0.9, ρ_2=0.42.

Example 1. Evaluation of the U235 fission cross-section in the range 1 – 2 MeV with taking USU into account be different techniques. Experimental data

- **19 experiments, 85 measurements at 7 neutron energies - nodes (1, 1.1, 1.25, 1.4, 1.6, 1.8, 2.0 MeV)**
- **the cross-section is relatively flat in the energy range**
- **8 experiments cover all the energy range**
- **experimental cross-section uncertainties consist of statistical and systematic components; the latter one is represented by the normalization uncertainty**
- **the normalization uncertainty exceeds the statistical one essentially to provide relatively strong correlation over energy range**
- **unknown parameters to be evaluated – cross-sections at 7 nodes and their covariances**

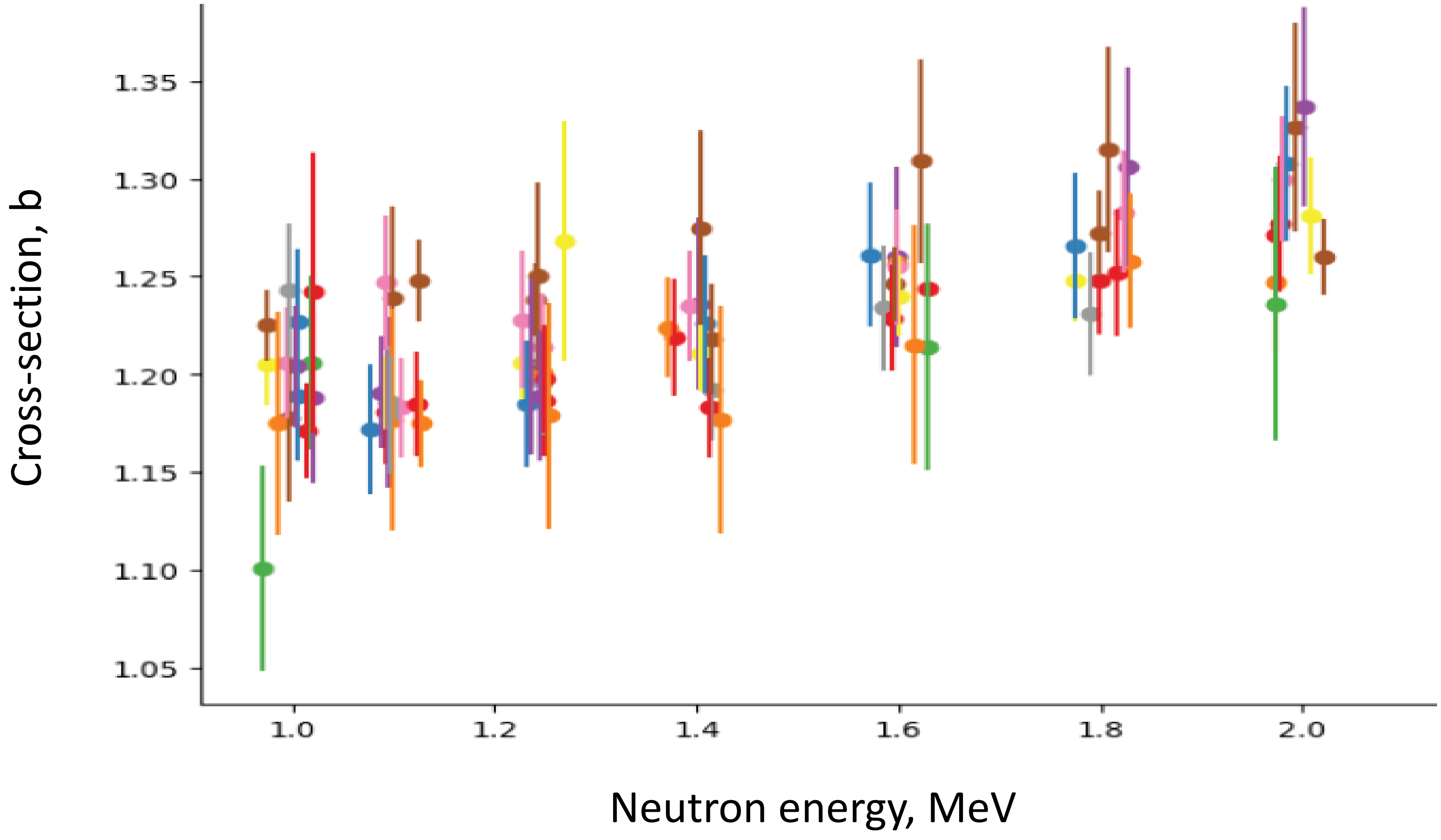
Example 1. Evaluation of the U235 fission cross-section in the range 1 – 2 MeV with taking USU into account by different techniques. List of experiments

Number	Reference	Energy range, MeV	Number of measurements
1	Wasson 1982	1.00 – 1.25	3
2	Carlson 1984	1.00 – 2.00	7
3	Kari 1978	1.00 – 2.00	7
4	Kaeppeler A 1972	1.10 – 1.25	2
5	Kaeppeler B 1972	1.00 – 1.10	2
6	Barton 1976	1.00 – 2.00	7
7	White 1965	1.00 – 1.00	1
8	Szabo 1970	1.00 – 1.00	1
9	Szabo 1973	1.00 – 2.00	7
10	Carlson 1978	1.00 – 2.00	7

Example 1. Evaluation of the U235 fission cross-section in the range 1 – 2 MeV with taking USU into account by different techniques. List of experiments (continued)

Number	Reference	Energy range, MeV	Number of measurements
11	Czirr 1976	1.00 – 2.00	7
12	Poenitz 1977	1.10 – 1.80	5
13	Poenitz A 1974	1.00 – 2.00	7
14	Poenitz B 1974	1.00 – 2.00	7
15	Yan 1975	1.00 – 1.00	1
16	Diven A 1957	1.00 – 1.60	5
17	Diven B 1957	1.25 – 1.25	1
18	Allen 1957	1.00 – 2.00	3
19	Carlson 1991	1.10 – 2.00	6

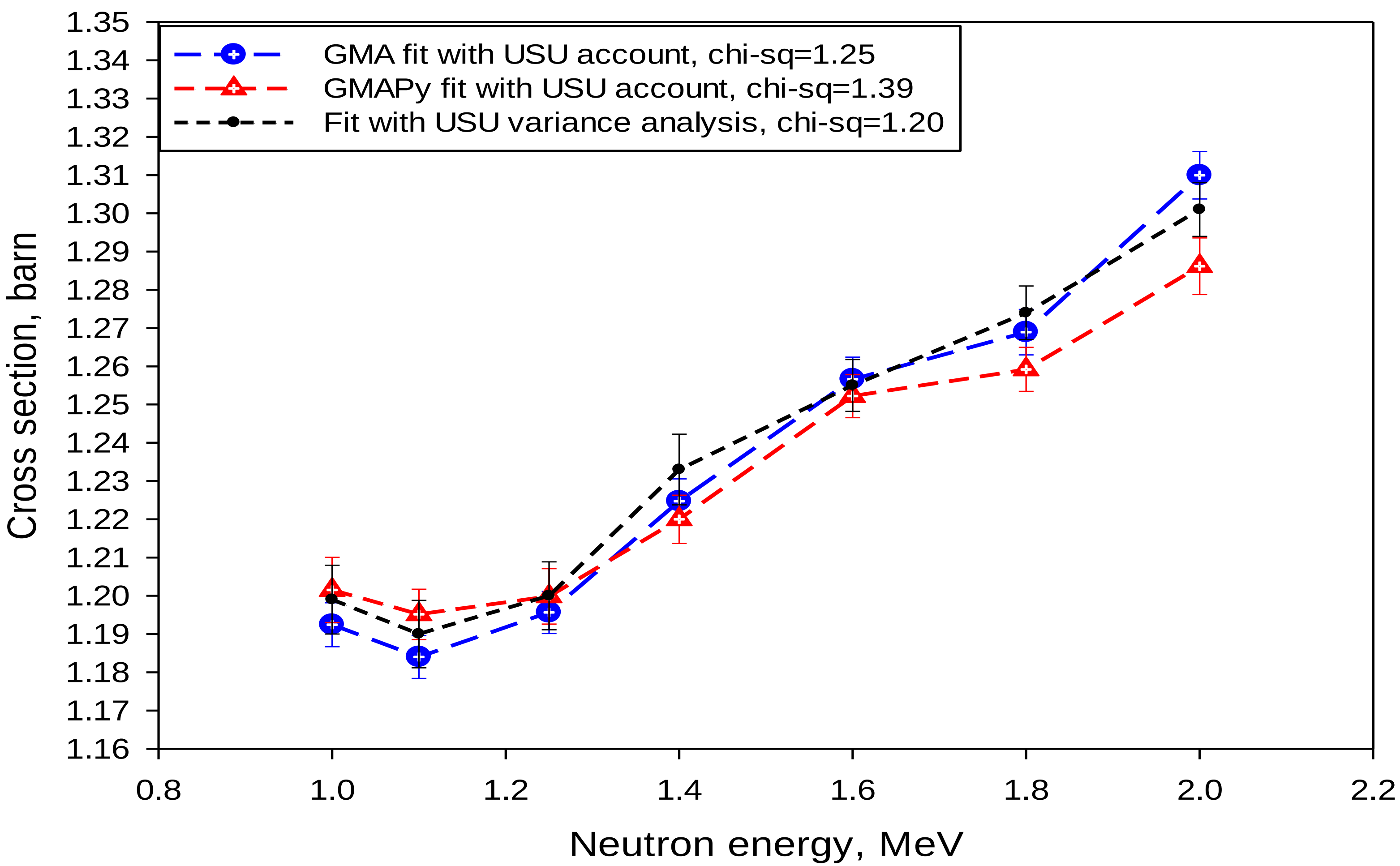
Example 1. Evaluation of the U235 fission cross-section in the range 1 – 2 MeV with taking USU into account by different techniques. Experimental data



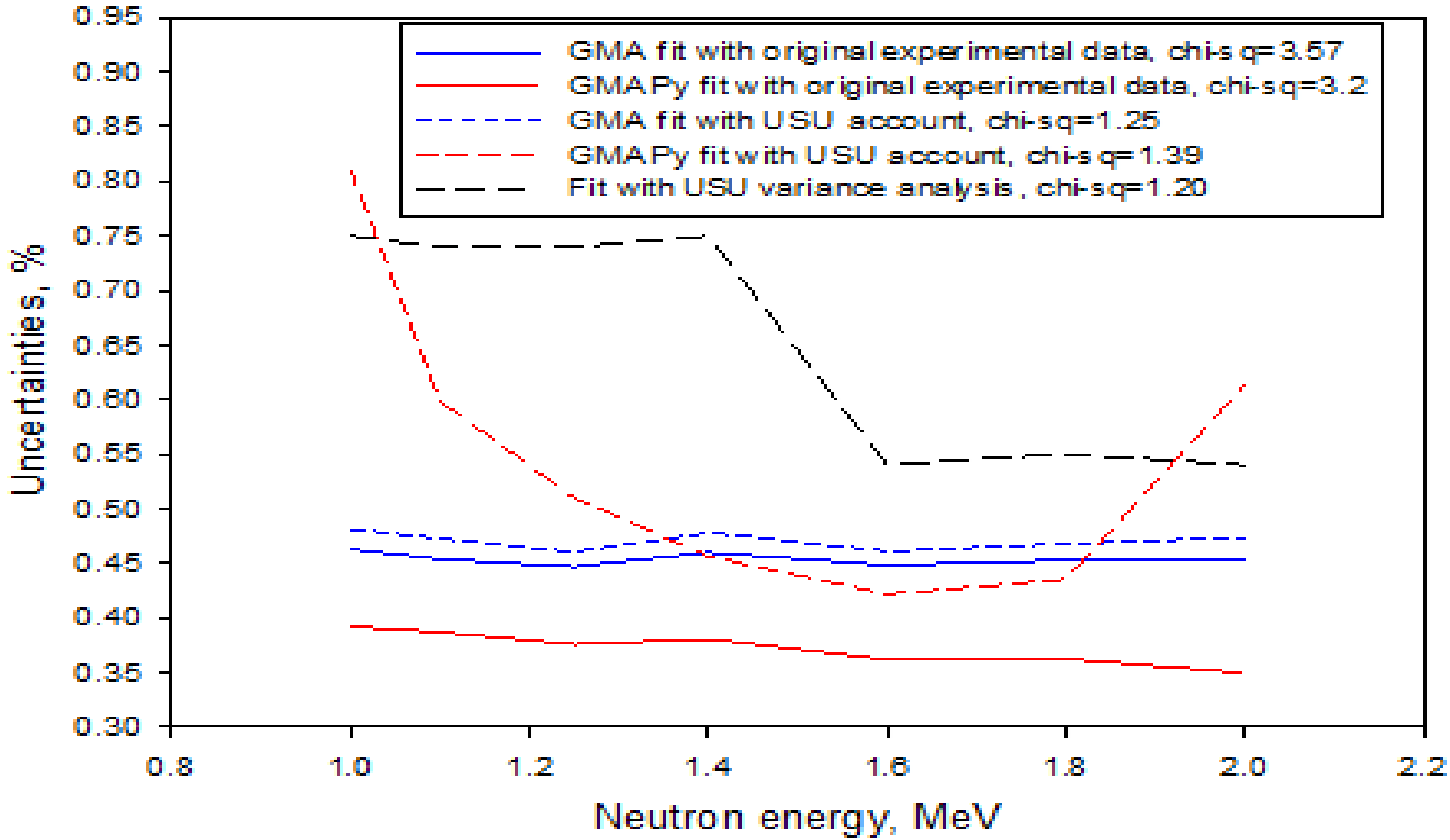
Example 1. Evaluation of the U235 fission cross-section in the range 1 – 2 MeV with taking USU into account by different techniques. Evaluated cross-sections (b) and their uncertainties (%)

Energy, MeV	GMA	GMA+ USU (ad-hoc)	GMAPy+USU (MC sampling)	Pade2+USU (variance analysis)
1.0	1.1980 ± 0.46	1.1924 ± 0.48	1.1957 ± 0.81	1.1990 ± 0.75
1.1	1.1917 ± 0.45	1.1840 ± 0.47	1.1943 ± 0.60	1.1905 ± 0.74
1.25	1.2008 ± 0.45	1.1956 ± 0.46	1.2052 ± 0.51	1.2002 ± 0.74
1.4	1.2256 ± 0.46	1.2247 ± 0.48	1.2193 ± 0.46	1.2260 ± 0.75
1.6	1.2598 ± 0.45	1.2566 ± 0.46	1.2518 ± 0.42	1.2552 ± 0.54
1.8	1.2709 ± 0.45	1.2690 ± 0.47	1.2649 ± 0.44	1.2744 ± 0.55
2.0	1.3014 ± 0.45	1.3100 ± 0.47	1.2866 ± 0.61	1.3010 ± 0.54

Example 1. Evaluation of the U235 fission cross-section in the range 1 – 2 MeV with taking USU into account by different techniques. Evaluated cross-sections



Example 1. Evaluation of the U235 fission cross-section in the range 1 – 2 MeV with taking USU into account by different techniques. Uncertainties of the evaluated cross-sections



Example 1. Evaluation of the U235 fission cross-section in the range 1 – 2 MeV with taking USU into account by different techniques. Comparison of integral uncertainties

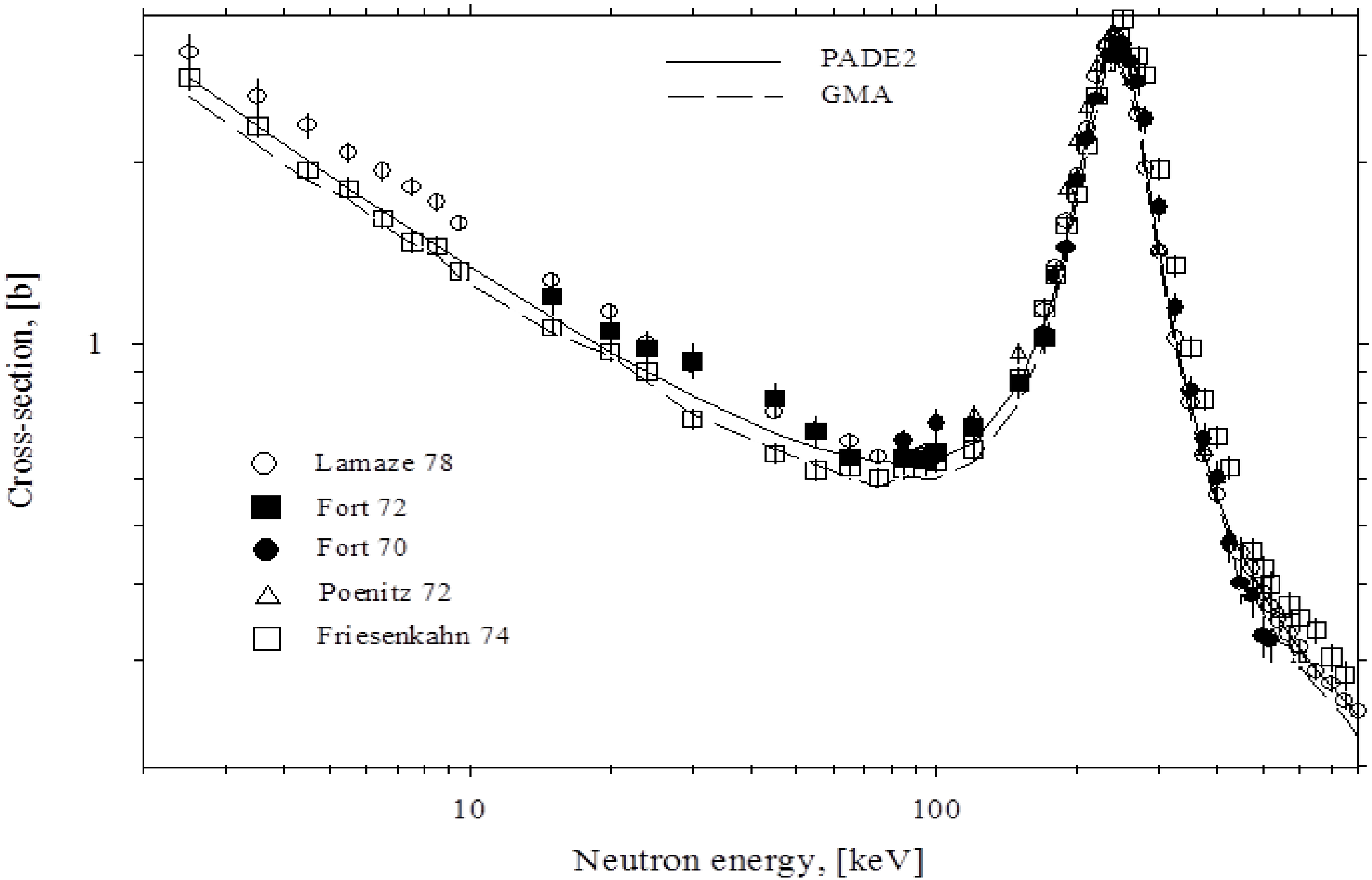
	GMA	GMA+ USU (ad-hoc)	GMAPy+USU (MC sampling)	Pade2+USU (variance analysis)
$\sqrt{tr(C)}$, b	1.485 - 2	1.537 - 2	1.828 - 2	2.158 - 2
$\sqrt{det(C)}, b^7$	1.537 - 18	3.022 - 18	1.263 - 16	1.921 - 17

- Trace and determinant of covariance matrix are integral characteristics providing additional uncertainty information for the evaluated data
- Taking USU into account by different techniques leads to increasing both the differential and integral uncertainties of the evaluated cross-sections
- There isn't a method that provides uniquely the best result for the entire set of integral characteristics

Example 2. Evaluation of the Li6(n,t) reaction cross-section in the range 2.5 – 800 KeV without taking USU into account

- 5 experiments (Fort 70, Poenitz 72, Fort 72, Friesenkahn 74, Lamaze 78)
- 1 resonance
- 2 experiments cover all the energy range
- GMA and PADE2 (9 parameters) calculations were carried out
- the experimental and evaluated data were folded in 9 energy groups; the group cross-sections and their covariances (for the experimental and evaluated data) were calculated
- integral characteristics for the covariance matrices were calculated and compared

Example 2. Evaluation of the Li6(n,t) reaction cross-section in the range 2.5 – 800 KeV without taking USU into account. Experimental and evaluated data



Example 2. Evaluation of the Li6(n,t) reaction cross-section in the range 2.5 – 800 KeV without taking USU into account.
Limits of energy groups for folding pointwise cross-sections

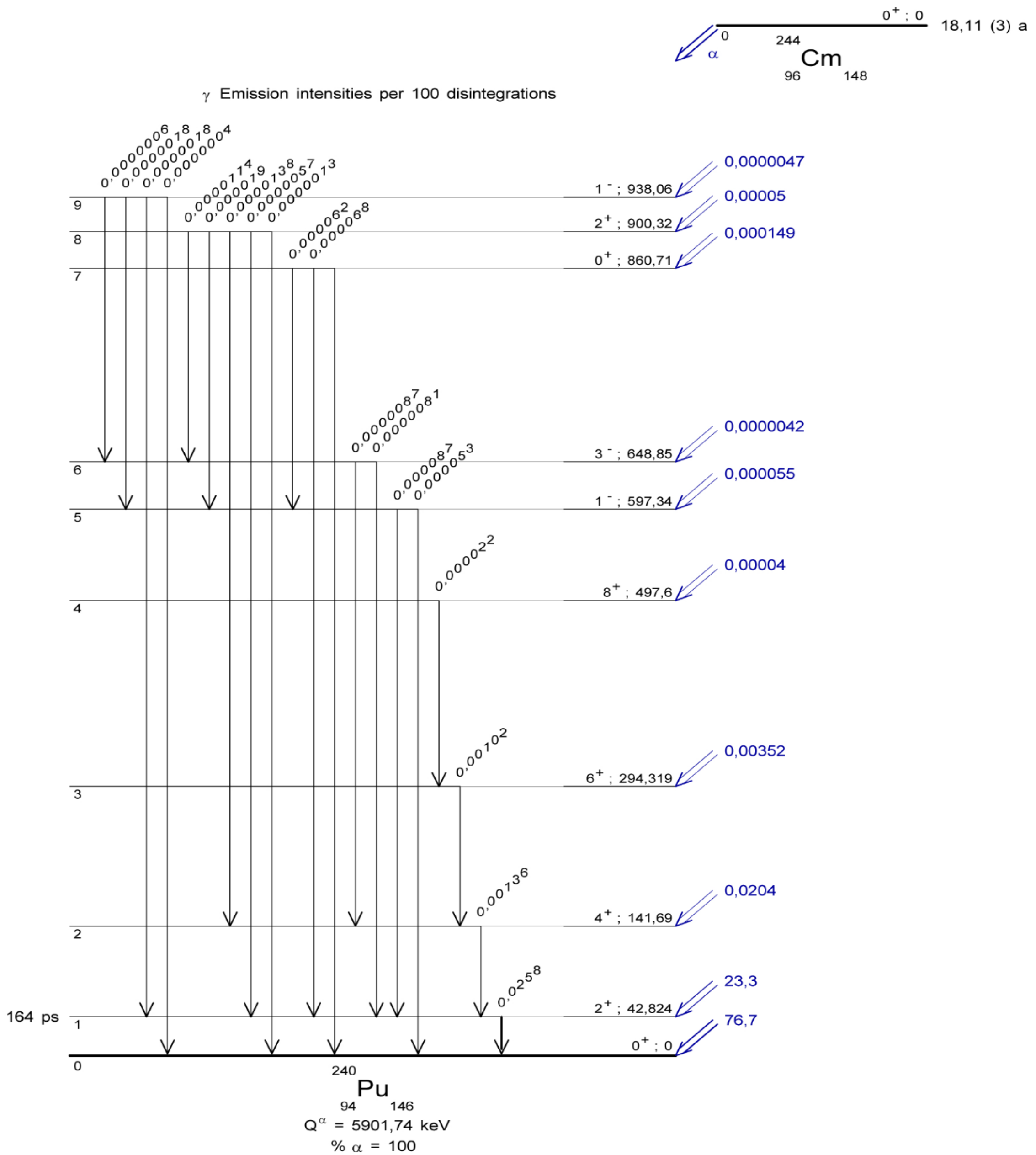
Number	Limits, keV	Number	Limits, keV
1	2.50 – 8.50	6	245 - 300
2	8.50 – 45.0	7	300 - 425
3	45.0 – 100	8	425 - 570
4	100 – 200	9	570 - 800
5	200 - 245		

Example 2. Evaluation of the Li6(n,t) reaction cross-section in the range 2.5 – 800 KeV without taking USU into account. Comparison of integral and pointwise (δ) cross-section uncertainties

	experiment	GMA	Pade2
$\sqrt{tr(C)}$, b	6.542 - 2	5.138 - 2	2.305 - 2
$\sqrt{det(C)}, b^9$	4.775 - 19	1.253 - 19	1.098 - 19
δ, %	4.04	2.12	1.17

- As expected both the integral and differential (pointwise) uncertainties of measured cross-sections exceed the uncertainties of evaluated cross-sections

Example 3. Evaluation of alpha emission probabilities in Cm-244 decay



Example 3. The evaluated Cm-244 alpha emission probabilities for the most intense transitions from different evaluations

N	E(α), keV	[1]	DDEP	ENDF/B-VII.1	JEFF-3.1
0	*5805*	*76.76 (10)*	*76.7 (4)*	*76.9 (1)*	*76.6 (1)*
1	*5763*	*23.21 (10)*	*23.3 (4)*	*23.1 (1)*	*23.4 (1)*
2	*5665*	*0.0204(6)*	*0.0204(15)*	*0.0204(15)*	*0.027(3)*

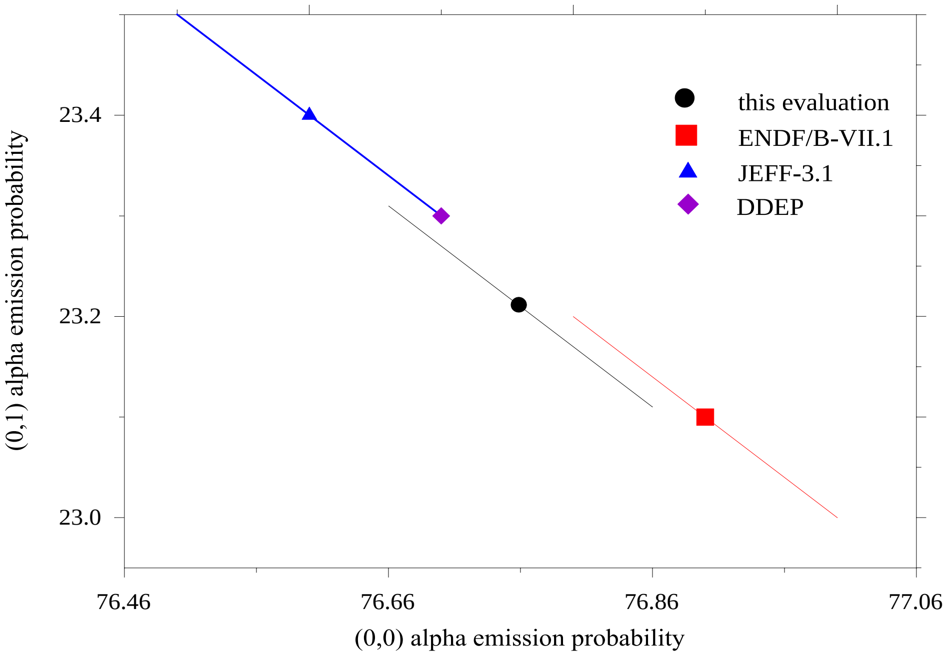
- All the evaluations look consistent within declared uncertainties

[1] Applied Radiation Isotopes v.109, p.164, 2016

Example 3. Correlation matrix of the Cm-244 alpha emission probabilities (in percent)

α-in-dex	0	1	2	3	4	5	6	7	8	9
0	100									
1	-99.9	100								
2	0	0	100							
3	0	0	5	100						
4	0	0	0	0	100					
5	0	0	3	60	0	100				
6	0	0	0	12	0	14	100			
7	0	0	-5	0	0	18	6	100		
8	0	0	4	69	0	71	4	32	100	
9	0	0	0	15	0	3	11	7	18	100

Example 3. Confidence regions of the evaluated Cm-244 (0,0) and (0,1) alpha emission probabilities



- in spite of consistency of single evaluations for the (0,0) and (0,1) absolute emission probabilities the evaluations (as 2-dimensional vectors) are inconsistent since the confidence regions haven’t common areas
- consideration of uncertainties for the components of the evaluated multidimensional vector separately from correlations can lead to false conclusions

Statistical invariants. Description of model

The measurements $y_{i_k}^k$ are assumed to be a sum of a model function $f(x_{i_k}^k, \vec{\theta})$ and random experimental errors, $\varepsilon_{\mathbf{i_k}}^{\mathbf{k}}$

$$y_{i_k}^k = f(x_{i_k}^k, \vec{\theta}) + \varepsilon_{i_k}^k, \quad i_k = 1, \ldots, n_k, \quad k = 1, \ldots, M,$$

with mathematical expectation

$$E\varepsilon_{i_k}^k = 0$$

and covariances ($V > 0$)

$$cov(\varepsilon_{i_k}^k, \varepsilon_{j_l}^l) = V_{ij}^k \delta_{kl},$$

n_k - the number of measurements in the experiment k, $\sum_k n_k = N$,

M – the number of experiments. The model function $f(x, \vec{\theta})$ is is a linear one

$$f(x, \alpha\vec{\theta}_1 + \beta\vec{\theta}_2) = \alpha f(x, \vec{\theta}_1) + \beta f(x, \vec{\theta}_2)$$

The unknown parameters of the model: $\theta_1, \ldots, \theta_L$.

Statistical invariants. LSM - solution

In case of linear model function the LSM formulae for an estimation of unknown vector of parameters $\hat{\vec{\theta}}$ and its covariance matrix W are well known

$$\hat{\vec{\theta}} = (X^t V^{-1} X)^{-1} X^t V^{-1} \vec{y}$$

$$W = (X^t V^{-1} X)^{-1}$$

where X – matrix of sensitivity coefficients of the model function relative to the parameters

Covariance matrix R of evaluated values of the model function can be calculated as

$$R = XWX^t$$

Statistical invariants. Interpretation of the evaluation process

- **As known from classical mechanics conserving values (for example, energy of closed system or other integrals of motion) are of special importance for analysis of *n* – particle system**

- **set of the experimental data y_i with covariances V_{ij}, *i* = *1,…,n* can be interpreted as a system of *n* particles with coordinates y_i; the interaction between particles is described by the values V_{ij}**

- **in turn, statistical processing can be interpreted as a transition of the *n* – particle system from one state $\left(y_i, V_{ij}\right)$ to another one $\left(\hat{\vec{y}}_i, R_{ij}\right)$**

- **so, it is reasonable to search a characteristics of the system which conserve at transition**

Statistical invariants (conservation laws)

For a **linear** model function there are **strict** relationships between the characteristics of the system in original and final states (for **nonlinear** model function the relationships are **approximate**)

$$\sum_i c_i \hat{y}_i = \sum_i c_i y_i \qquad \sum_i \sum_j c_i R_{ij} c_j = \sum_i c_i V_{ij} c_j$$

where weights c_i are determined as follows

$$c_i = \frac{\sum_j (V^{-1})_{ji}}{\sum_k \sum_j (V^{-1})_{jk}}$$

Thus, the evaluated values $\hat{y}_i$ and their covariances R_{ij} are result of a **redistribution** of the experimental values y_i and their covariances V_{ij} .

The redistribution is managed by the weights c_i .

Statistical invariants. Meanings

The invariants have a clear statistical meanings

$$\sum_i c_i \hat{y}_i = \sum_i c_i y_i$$

Average (weighted in special way) value of the model function in the range under consideration

$$\sum_i \sum_j c_i R_{ij} c_j = \sum_i c_i V_{ij} c_j$$

Variance of the average (weighted in special way) value of the model function in the range under consideration

Statistical invariants.
Enequalities imposing restrictions on the experimental covariances

$$\frac{\sum_j (V^{-1})_{ji}}{\sum_k \sum_j (V^{-1})_{jk}} \geq 0$$

from positivity of weights

$$\sum_k \sum_j (V^{-1})_{jk} > 0$$

from positivity of variance

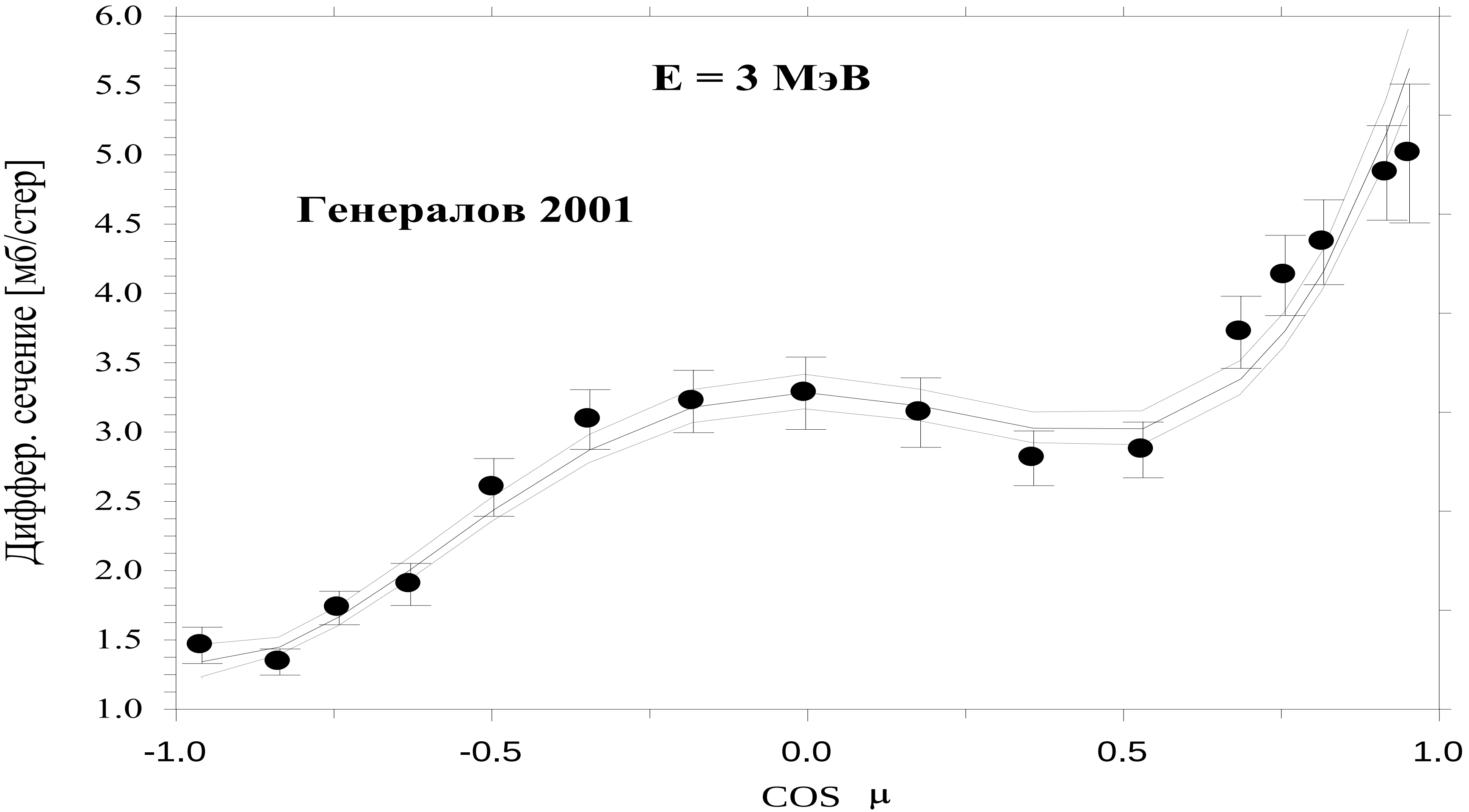
of the physical quantity

Statistical invariants. Example.
Evaluation of the 9Be(d,α0) differential reaction cross-section at deutron energy 3 MeV. Results of measurements [2]

angle, grad	c-section, mb/ster	Uncertainty,%	Angle, grad	c-section, mb/ster	Uncertainty,%
17.7	5.01	10	90.2	3.28	8
23.5	4.87	7	100.4	3.22	7
35.2	4.37	7	110.2	3.09	7
40.9	4.13	7	119.8	2.60	8
46.7	3.72	7	129.0	1.90	8
57.9	2.87	7	137.9	1.73	7
69.0	2.81	7	146.7	1.34	7
79.7	3.14	8	163.5	1.46	9

[2] Generalov L.N. et al., “LI Meeting on Nuclear Spectroscopy and Nuclear Structure”, P. 187. Sarov, RFNC-VNIIEF, 2001 [in Russian], EXFOR F0530

Statistical invariants. Example.
Evaluation of the 9Be(d,α0) differential reaction cross-section at deutron energy 3 MeV. Plot of the experimental data



Statistical invariants. Example.

Evaluation of the 9Be(d,α0) differential reaction cross-section.

Evaluated coefficients of Legendre polynomial

$$\sigma(\mu,E)=\sum_{l=0}^{N}\theta_N^l P_l(\mu)$$

θ_4^0	θ_4^1	θ_4^2	θ_4^3	θ_4^4
2.968	1.464	0.01839	1.020	0.8686

Statistical invariants. Example.

Evaluation of the 9Be(d,α0) differential reaction cross-section.

Covariances (x1000) of evaluated coefficients of Legendre polynomial

$$\sigma(\mu, E) = \sum_{l=0}^{N} \theta_N^l P_l(\mu)$$

	Number	0	1	2	3	4
θ_4^0	0	3.517				
θ_4^1	1	1.770	7.577			
θ_4^2	2	-1.874	4.912	17.55		
θ_4^3	3	1.238	0.3945	6.929	23.78	
θ_4^4	4	2.701	0.1747	-0.7937	10.96	24.58

Evaluation of the 9Be(d,α0) differential reaction cross-section.

Checking the statistical invariants

$\sum_i c_i y_i, \frac{mb}{ster}$	$\sum_i c_i \hat{y}_i, \frac{mb}{ster}$	$\sum_i \sum_j c_i V_{ij} c_j, \frac{mb^2}{ster^2}$	$\sum_i \sum_j c_i R_{ij} c_j, \frac{mb^2}{ster^2}$
2.260	2.260	2.091-3	2.091-3

Summary

- Input experimental data (results of measurements and their covariances) **predetermine** the evaluated data and their covariances calculated by the LSM for **any linear** model function;
- As follows from the conservation laws **relative decreasing (increasing) uncertainties** of the evaluated data leads to **pumping** uncertainty information into the off-diagonal covariances
- strict relationships between input experimental data and output evaluated data, restrictions imposed to the covariances of the experimental errors provide verification both the final and intermediate results of calculations
- Integral uncertainties of the random vector (trace and determinant of covariance matrix) provide **additional** uncertainty information for the evaluated data
- As seen today the adequate processing of USU (inconsistent experimental data) is a key for getting reliable uncertainty information for the evaluated data