Yelow colored: need to be confirmed by SG33 members.
Pink colored: Typo or correction. Nov.29, 2012 M.Ishikawa

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APPENDIX

Teaching Example of Adjustment Methods Features

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I. Introduction

In the cross-section adjustment procedure, various kinds of differential and integral parameters affect the adjusted results with very complicated manners. The objective of this appendix is to illustrate the physical meaning of each parameter used in the adjustment, by means of dealing with a very simple problem.

II. Theory of Cross-section Adjustment

Bayes'

The cross-section adjustment methodology is based on the Bayesian theory and the generalized least-square technique (for example, Ref.1), where all related information including cross-section covariance, sensitivity coefficients, integral C/E (Calculation/Experiment) values, experimental and analytical modeling errors, is synthesized with physical consistency. Based on the Bayes theorem, i.e., the conditional probability estimation method, the posterior probability that a cross-section set, ***T***, is true, is maximized under the condition that the information of integral experiments, ***R***, is obtained:

$$J(T) = (T-To)^t M^{-1}(T-To) + [Re-Rc(T)]^t[Ve+Vm]^{-1}[Re-Rc(T)] \qquad \text{- - - (A.1)}$$

where,

- ***J(T)***: An error function targeted for the combined set of differential and integral data,
- ***To*** : A prior cross-section set before adjustment,
- ***M*** : Covariance of the prior cross-section set ***To*** before adjustment,
- ***Re*** : Measured values of the integral experiment set, and,
- ***Rc(T)*** : Analytical values of the integral experiment set obtained with the cross-section set ***T***,
- ***Ve*** : Experimental error matrix of an integral experiment set ***Re***,
- ***Vm*** : Analytical modeling error matrix of the analyzed integral experiment set ***Rc***.

In order to minimize the error function ***J(T)***, its differentiation with respect to ***T*** is required to be zero.

$$dJ(T)/dT = 0. \qquad \text{- - - (A.2)}$$

After analytical derivations with the linearity assumption between ***Rc(T)*** and ***T***, the posterior cross-section set, ***T'***, and its covariance, ***M'***, after adjustment are obtained as follows:

$$T' = To + MG^t[GMG^t+Ve+Vm]^{-1}[Re-Rc(To)] \qquad \text{- - - (A.3)}$$

$$M' = M - MG^t[GMG^t+Ve+Vm]^{-1}GM \qquad \text{- - - (A.4)}$$

where,

G : Sensitivity coefficients of an integral parameter, ***R***, with respect to ***T***, that is,

$$G = (dR/R)/(d\,T/T). \qquad \text{- - - (A.5)}$$

The minimized $\boldsymbol{J(T)}$ function is generally called the minimized chi-square, $\chi^2_{\mathbf{min}}$ (see Ref.2, p.221). Note that the second term of the right-hand side in Eq.(A.6) applies the optimized posterior analytical values of integral parameters, $\boldsymbol{Rc(T')}$, on the contrary, the prior values, $\boldsymbol{Rc(To)}$, is used in the right-hand side of Eq.(A.7).

$$\chi^2_{\mathbf{min}} = \boldsymbol{(T'-To)^t M^{-1}(T'-To) + [Re-Rc(T')]^t[Ve+Vm]^{-1}[Re-Rc(T')]} \quad \text{- - - (A.6)}$$
$$= \boldsymbol{[Re-Rc(To)]^t[GMG^t + Ve+Vm]^{-1}[Re-Rc(To)]} \quad \text{- - - (A.7)}$$

where,

$$\boldsymbol{Rc(T') = Rc(To)+G(T'-To)} \quad \text{- - - (A.8)}$$

The prior and posterior uncertainty of integral parameters induced by the cross-section errors are calculated with $\boldsymbol{GMG^t}$ and $\boldsymbol{GM'G^t}$, respectively. We here find some features of the posterior cross-section-induced error, $\boldsymbol{GM'G^t}$, observing a product of Eq.(A.4) multiplied by the sensitivity $\boldsymbol{G}$ from the left- and right-sides with some approximations:

$$\text{If } \boldsymbol{GMG^t << Ve+Vm}, \text{ then } \boldsymbol{T' \fallingdotseq To} \text{ and } \boldsymbol{GM'G^t \fallingdotseq GMG^t} \quad \text{- - - (A.9)}$$
$$\text{If } \boldsymbol{GMG^t >> Ve+Vm}, \text{ then } \boldsymbol{GM'G^t \fallingdotseq Ve+Vm} \quad \text{- - - (A.10)}$$
$$\text{If } \boldsymbol{GMG^t \fallingdotseq Ve+Vm}, \text{ then } \boldsymbol{GM'G^t \fallingdotseq 1/2 \times GMG^t} \quad \text{- - - (A.11)}$$

III. Simulation of Adjustment Procedure

Here, we treat a very simple data set to simulate the adjustment procedure. This system is comprised of three cross-sections (**s1**, **s2** and **s3**) and two integral parameters (**R1** and **R2**).

(Standard Case)

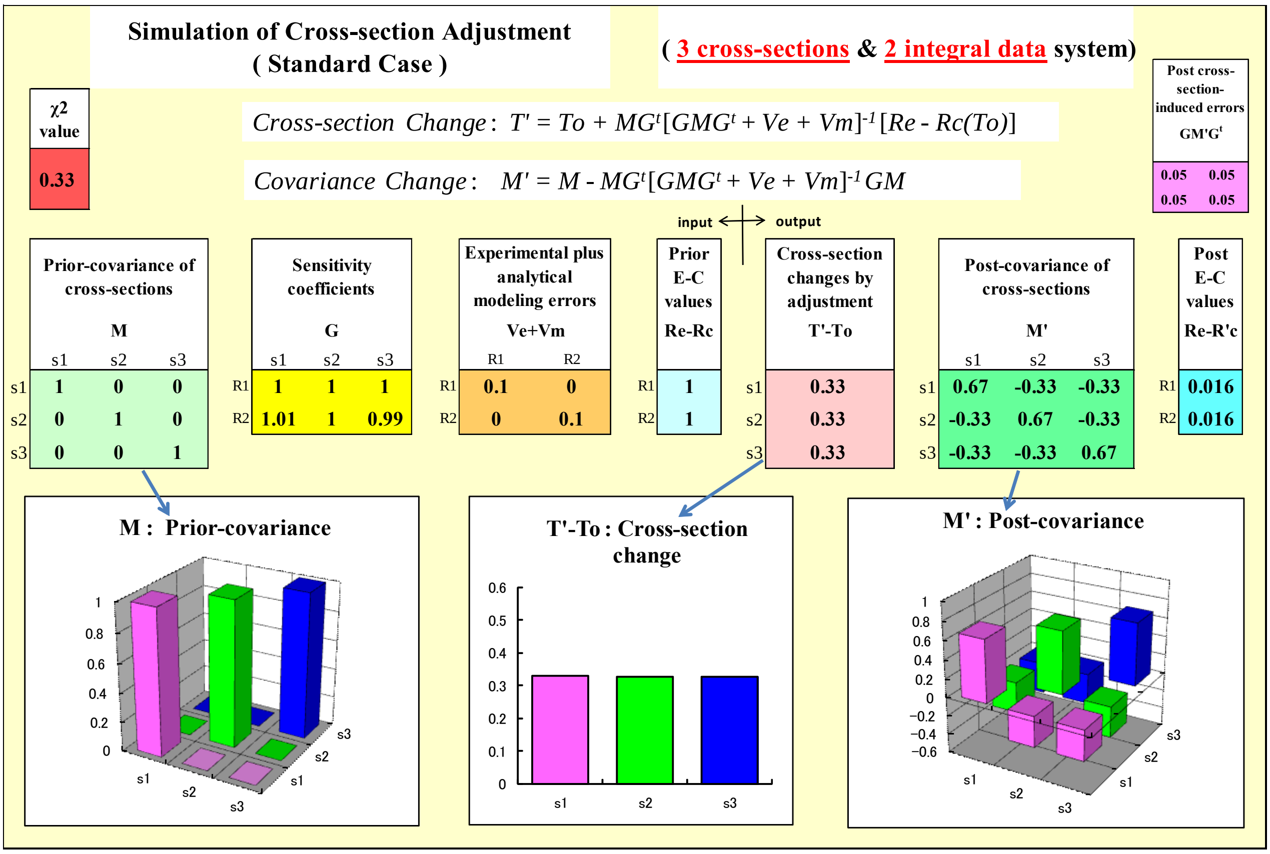
In **Fig. A.0**, the input set of the standard case and the results of adjustment, i.e., output, are summarized in the form of both tables and graphs. The cross-section covariance is composed of a 3-by-3 square matrix. The prior values of the matrix components are given as 1.0 for the diagonal terms, that is, the variance (=cov(x_i, x_i)) or the square of the standard deviation (=[std(x_i)]^2). For the non-diagonal terms of the matrix (=cov(x_i, x_j), $i \neq j$), the values of 0.0 are given, that is, there are no-correlations among three cross-sections. The sensitivity is also a matrix with 2-by-3 elements. The sensitivity coefficients of integral parameter **R1** with respect to cross-sections are set as 1.0 for all three cross-sections, and those of **R2** to cross-sections **s1**, **s2** and **s3** are 1.01, 1.0 and 0.99, respectively. Namely, the sensitivity coefficient vectors of **R1** and **R2** are set to be very similar, but not completely identical to avoid mathematical irregularity. The error of integral parameters, that is, the summation of experimental error ***Ve*** and analytical modeling error ***Vm***, is a 2-by-2 matrix. The matrix elements are given as 0.1 for the diagonal terms, and zero for non-diagonal terms. These values mean there is no correlation between the error of **R1** and **R2**, and the integral error values are extremely small compared with the cross-section-induced errors, $\boldsymbol{GMG^t}$, which corresponds to the case of Eq.(A.10). The prior **E-C** value vector is set as 1.0 for both **R1** and **R2**.

The $\chi^2_{\mathbf{min}}$ value of this standard case is calculated as 0.33 using Eq.(A.7). From the statistical viewpoint, the $\chi^2_{\mathbf{min}}$ value is expected to be close with the degree of freedom in the dataset, that is, the number of the integral parameters. Though the value of 0.33 is quite smaller than 2, it is no matter for this simulations[1].

[1] If one would like to force the $\chi^2_{\mathbf{min}}$ value to be approximately the degree of freedom, it is easily attained. Setting the prior **E-C** values as 2.5 for both **R1** and **R2** will make $\chi^2_{\mathbf{min}}$ to be the value of 2.05. However, we avoid it here since the adjusted results will become difficult to understand intuitively.

As the consequence of the adjustment operation, first, all cross-sections are changed by +0.33. When one multiply the cross-section alterations by the sensitivity coefficients as Eq.(A.8), the posterior **E-C** values become approximately zero for both integral parameters **R1** and **R2**, which can be expected from Eq.(A.10). It is also reasonable that the values of cross-section alterations are same among **s1**, **s2** and **s3**. The variances and the sensitivity coefficients are practically identical among three cross-sections, therefore, the contribution from each cross-section must be equal as indicating in Eq.(A.3), if there is no correlations among cross-sections. Second, every diagonal-term of the posterior cross-section covariance decrease to a value of 0.67, which is just two-thirds of the prior variance. The important thing to be noticed here is that all non-diagonal terms of the posterior covariance shift to the negative values, -0.33 (= -0.49 as the correlation factor (= ρ_{ij}))[2] in this case. By observing Eq.(A.4), we guess the non-diagonal terms of the cross-section covariance would move to the negative direction, as well as the diagonal terms. The posterior cross-section-induced error matrix, $\boldsymbol{GM'G^t}$, is found very close to the integral parameter error matrix, $\boldsymbol{Ve+Vm}$, which is consistent with the prediction by Eq.(A.10). Note that the contributions to the reduction of the cross-section-induced error consist of one-third from the diagonal terms, and two-third from the non-diagonal terms.

Figure A.0 Simulation of Cross-section Adjustment (Standard Case)



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[2] Correlation factor between elements x_i and x_j: $$\rho_{ij} = \frac{\mathrm{cov}(x_i, x_j)}{std(x_i) \times std(x_j)} \quad \text{where,} \quad -1 \le \rho_{ij} \le +1$$

Hereafter, we change an input value of the standard case, one by one, to understand the effect of each parameter in the adjustment procedure.

(Case 1) Effect of Cross-section Standard Deviation (or Variance)

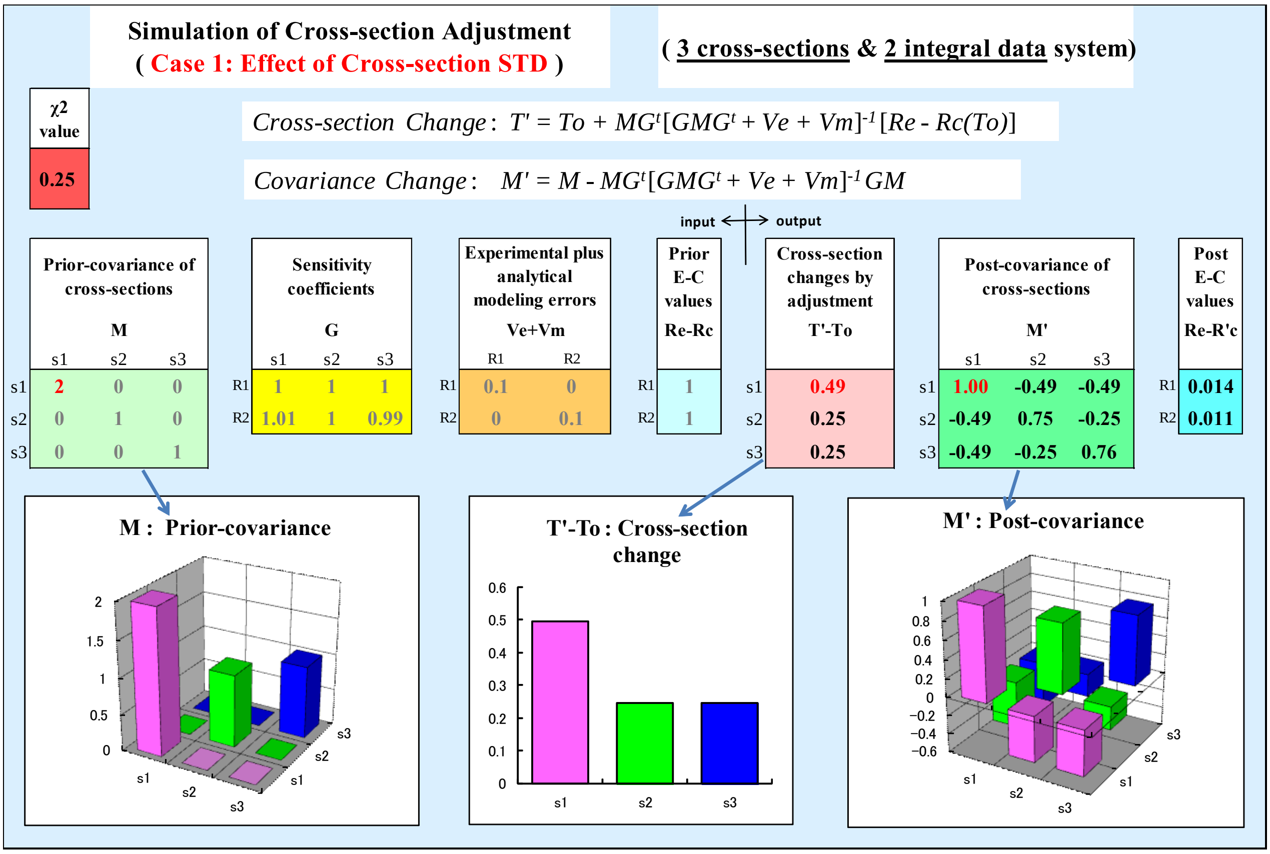
In **Fig. A.1**, the variance of the prior cross-section **s1** is changed to 2.0, which is twice of the standard case. The grey-colored figures in the input mean they are unchanged from the standard case.

The posterior **E-C** values are almost zeros like the standard case, but the contributions of cross-sections are quite different. The cross-section **s1** is altered by +0.49, which is roughly double with the value of other **s2** and **s3**, +0.25. From Eq.(A.3), the cross-section alteration rate, ***T'-To***, appears to be rather proportional with the value of covariance, ***M***, though the degree is somewhat mitigated by the denominator which includes ***M***. Actually, a cross-section with large uncertainty would tend to be altered significantly by the adjustment, if the its sensitivity is comparable with other cross-sections.

The posterior variance of the cross-section **s1** reduces to 1.0, which is a half of the prior value, 2.0, but the values of other **s2** and **s3** are around 0.75, which is three fourths of the prior. The non-diagonal terms of the posterior covariance also move to more negative for the elements related to **s1** than the other correlation between **s2** and **s3**. Converting the values of covariance elements to the correlation factors, the posterior ones are -0.57 between **s1** and **s2**, and -0.32 between **s2** and **s3**. In summary, the reduction of cross-section error is also significant for the cross-section with large uncertainty, as well as the cross-section alteration, when other conditions are same among cross-sections.

The χ^2_{min} value becomes 0.25 which is smaller than that of the standard case 0.33, since the denominator of Eq.(A.7) becomes large due to the prior covariance.

Figure A.1 Simulation of Cross-section Adjustment (Case 1)



(Case 2) Effect of Cross-section Correlation

In **Fig. A.2**, a strong positive correlation between the cross-sections **s1** and **s2** are given as +0.9, which is zero in the standard case. The other inputs are not changed.

The posterior **E-C** values are almost zeros like the standard case, but the contributions of cross-sections are quite different again. The cross-section **s1** and **s2** are altered by +0.39 both, which is double with that of **s3**, +0.20. If we gave a value of 2 to the variance of **s2** as well as **s1** as a modification of Case 1, practically comparable cross-section alterations with this Case 2 would be obtained. From these facts, we guess that giving the correlation among cross-sections would play a similar role to change their variances in some situations. In other expressions, the correlation in covariance would be also a kind of error values in the adjustment.

The posterior variances of the cross-sections **s1** and **s2** reduce to 0.25 for both, which is one-fourth of the prior value, while the posterior of uncorrelated **s3** is 0.80, the reduction of which is much smaller than those of correlated **s1** and **s2**. The non-diagonal terms of the posterior covariance between **s1** and **s2** still has a positive value of +0.15, but the reduction from the prior value is quite large. As the correlation factor values, the posterior one between **s1** and **s2** is +0.6, which reduces from the prior value, +0.9. The non-diagonal correlation factors related to the uncorrelated **s3** are -0.87, which is smaller in absolute than the value of the standard case -0.49. However, the quantitative trends of the posterior covariance do not seem easy to understand in this Case 2.

The χ^2_{min} value of Case 2 is 0.21 which is smaller than that of the standard case 0.33, due to the large prior covariance as well as Case 1.

Figure A.2 Simulation of Cross-section Adjustment (Case 2)

Simulation of Cross-section Adjustment
(Case 2: Effect of Cross-section Correlation)

(3 cross-sections & 2 integral data system)

χ2 value: 0.21

Cross-section Change: $T' = To + MG^t[GMG^t + Ve + Vm]^{-1}[Re - Rc(To)]$

Covariance Change: $M' = M - MG^t[GMG^t + Ve + Vm]^{-1}GM$

input ← → output

Prior-covariance of cross-sections M

	s1	s2	s3
s1	1	0.9	0
s2	0.9	1	0
s3	0	0	1

Sensitivity coefficients G

	s1	s2	s3
R1	1	1	1
R2	1.01	1	0.99

Experimental plus analytical modeling errors Ve+Vm

	R1	R2
R1	0.1	0
R2	0	0.1

Prior E-C values Re-Rc

R1	1
R2	1

Cross-section changes by adjustment T'-To

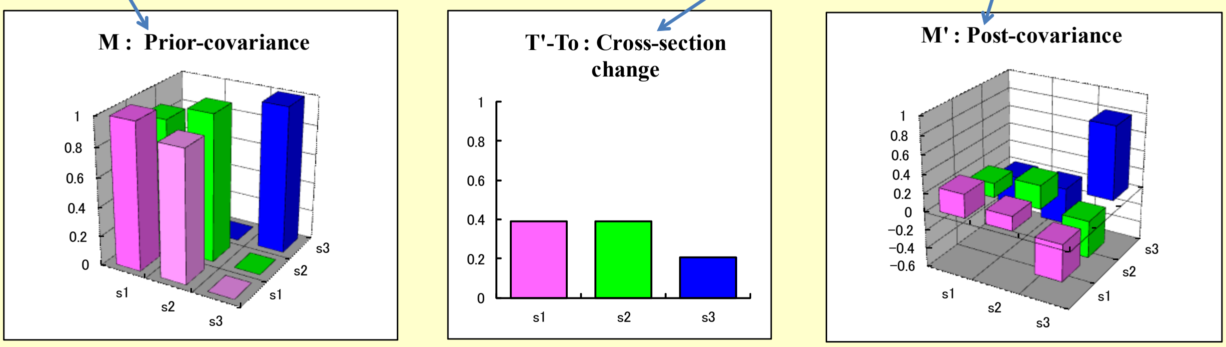
s1	0.39
s2	0.39
s3	0.20

Post-covariance of cross-sections M'

	s1	s2	s3
s1	0.25	0.15	-0.39
s2	0.15	0.25	-0.39
s3	-0.39	-0.39	0.80

Post E-C values Re-R'c

R1	0.011
R2	0.009



(Case 3) Effect of Sensitivity Coefficient

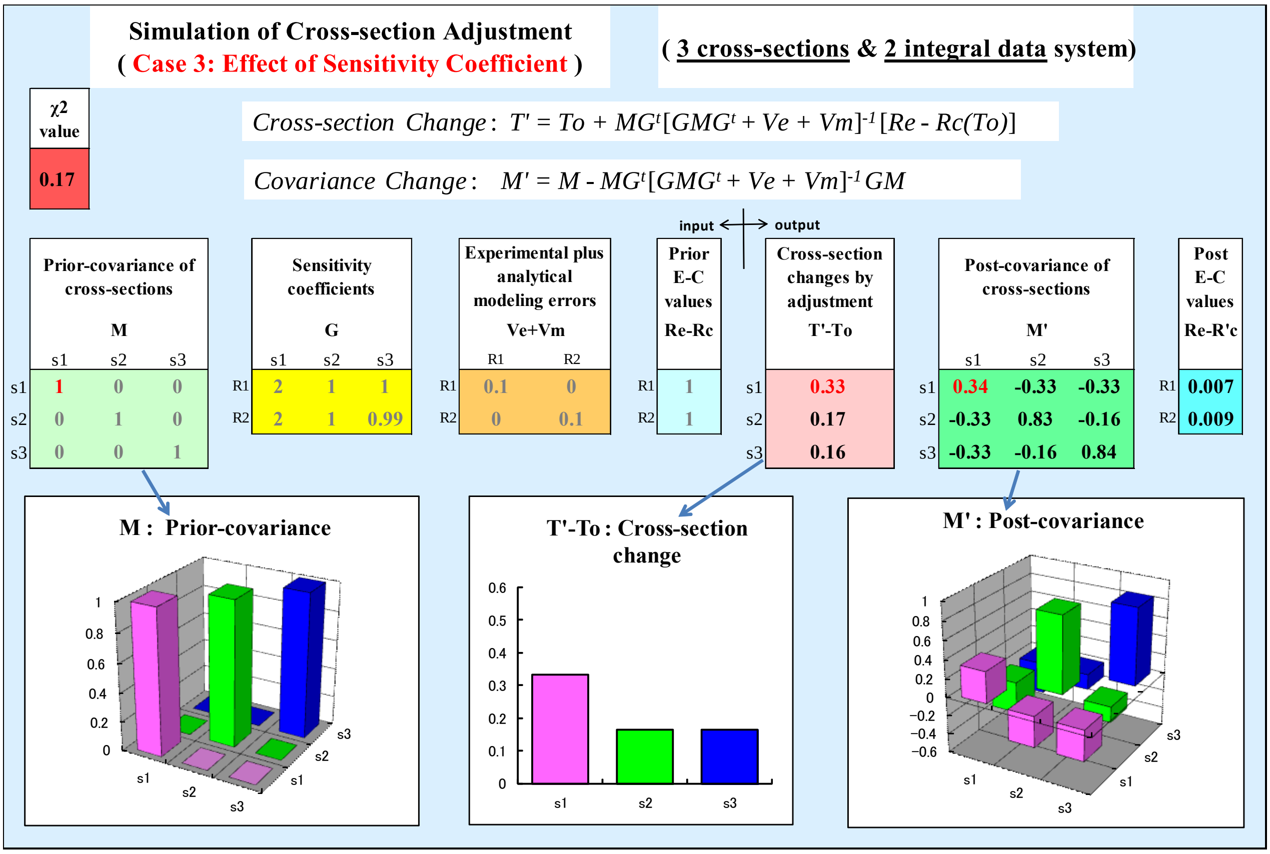
In **Fig. A.3**, the sensitivity coefficients of the integral parameters **R1** and **R2** with respect to the cross-section **s1** are made twice with those of the standard case. The other inputs are not changed.

The posterior **E-C** values are almost zeros like the standard case, but the contributions of three cross-sections are also different. The altered value of the cross-section **s1** is +0.33, which is roughly double with the value of the other **s2** and **s3**, around +0.16. From Eq.(A.3), the cross-section alteration rate, ***T'-To***, is suggested to be rather proportional with the value of sensitivity coefficients, ***G***, as well as the cross-section covariance, ***M***. In this Case 3, the contribution of **s1** to the **E-C** changes is 4-times larger than those of the other **s2** and **s3**. Coupling with Case 1 conclusion, a cross-section with large uncertainty and/or large sensitivity would tend to be altered significantly by the adjustment.

The posterior variance of the cross-section **s1** reduces to 0.34, which is one third of the prior value, but the values of other **s2** and **s3** are around 0.83, which is rather close to the prior. The non-diagonal terms of the posterior covariance also move to more negative for the elements related to **s1** than the other correlation between **s2** and **s3**. As the correlation factors, the posterior ones are -0.62 between **s1** and **s2**, and -0.20 between **s2** and **s3**. In summary, the reduction of cross-section uncertainty is significant for the cross-section with large sensitivity, as well as the cross-section alteration.

The χ^2_{min} value is 0.17 which is smaller than that of the standard case 0.33, since the denominator of Eq.(A.7) becomes large due to the sensitivity coefficients. Note that the sensitivity coefficients, ***G***, contributes to the accuracy of integral data as the square of the values with the term, $\boldsymbol{GMG^t}$.

Figure A.3 Simulation of Cross-section Adjustment (Case 3)



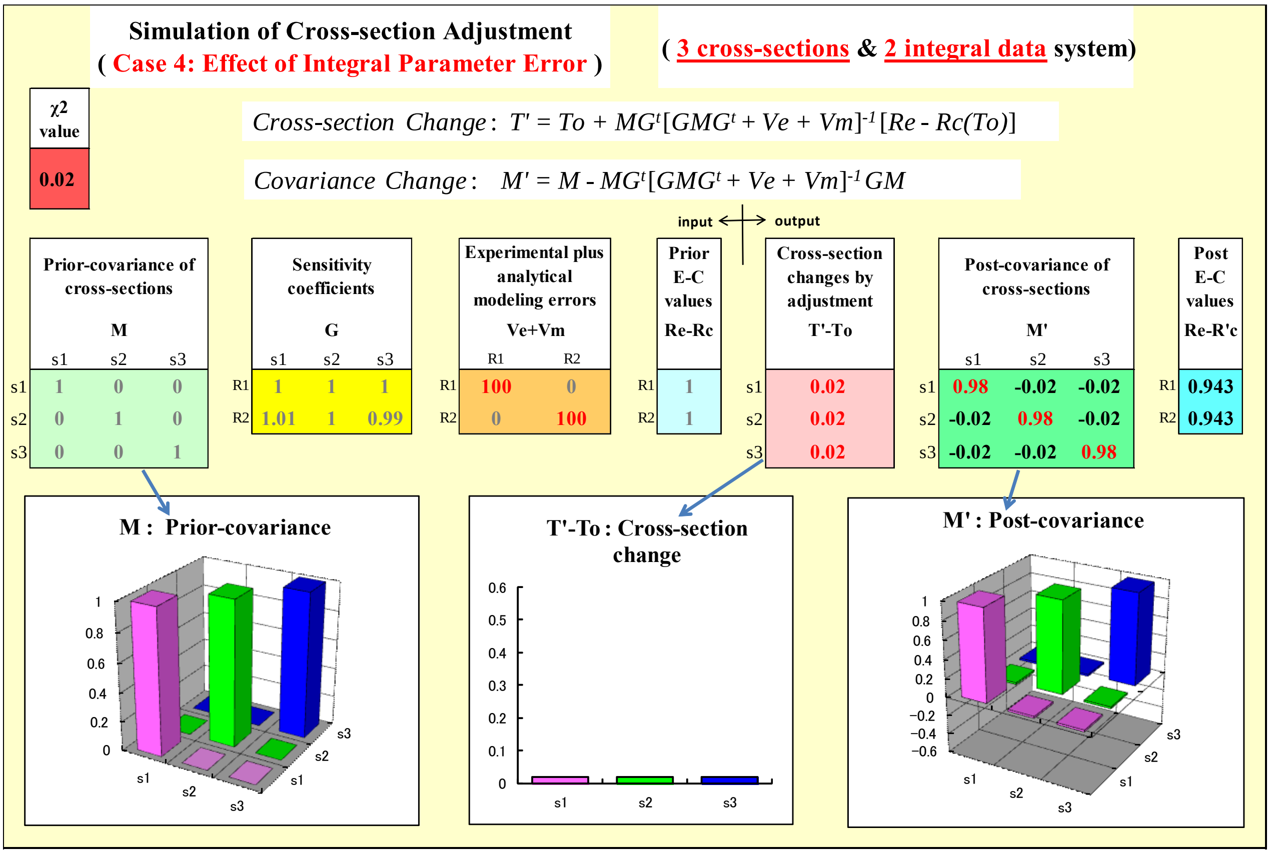
(Case 4) Effect of Integral Parameter Error

In **Fig. A.4**, the diagonal terms of the integral parameters error matrix, ***Ve+Vm***, are made extremely large for both **R1** and **R2** to be a value of 100, compared with those of the standard case, 0.1. The other inputs are not changed.

The posterior **E-C** values are 0.94 for both **R1** and **R2**, which is hardly altered from the prior values, 1.0. The cross-sections and their covariance hardly change by the adjustment either. These results are consistent with Eq.(A.9). When the integral parameters possess very large errors, ***Ve+Vm***, compared with the cross-section-induced error matrix, $\boldsymbol{GMG^t}$, these integral data have no influence to the adjusted results. In this Case 4, the posterior dataset is almost same as the prior. It should be emphasized that the integral data with large errors do no harm to the adjusted results, since they are simply ignored in the adjustment procedure. On the contrary, the integral data with too small errors which is improbable physically, must not to be adopted in the adjustment, since it will alter the posterior covariance (and related cross-sections) too much largely as guessed from Eq.(A.10).

The χ^2_{min} value is 0.02 which is much smaller than that of the standard case 0.33, since the denominator of Eq.(A.7) is extremely large.

Figure A.4 Simulation of Cross-section Adjustment (Case 4)



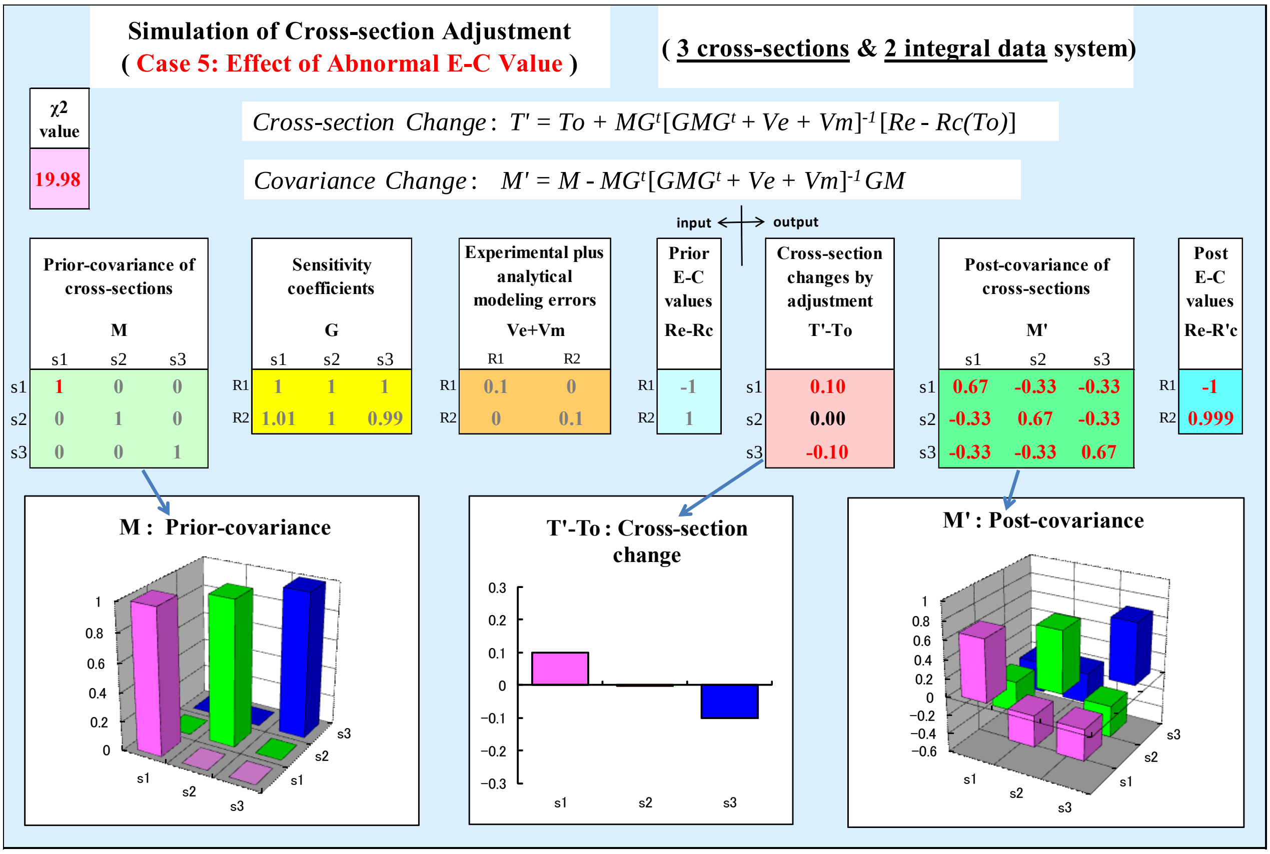
(Case 5) Effect of Abnormal E-C Value

In **Fig. A.5**, the **E-C** value of the integral parameter **R1** are changed to -1.0 from that of the standard case, +1.0. The other inputs including the **C-E** value of **R2** are not changed. Since the integral error matrix, ***Ve+Vm***, is sufficiently small compared with the prior cross-section-induced errors, $\boldsymbol{GMG^t}$, the prior **E-C** values are practically determined only by the cross-section errors. In addition, the sensitivity coefficients of both **R1** and **R2** are nearly identical here. Hence we judge that the prior **E-C** values of **R1** and **R2**, -1.0 and +1.0 are obviously inconsistent with each other. In other words, we should consider that there would be some serious mistakes to evaluate the value of **E** or **C** or ***Ve+Vm***, or everything in this Case 5.

The posterior **E-C** values are -1.0 for **R1**, and +0.999 for **R2**, which are hardly altered from the prior values. The posterior cross-section covariance ***M'*** is identical with the standard case, that is, +0.67 for the diagonal terms, and -0.33 for the non-diagonal. The posterior cross-section-induced error matrix $\boldsymbol{GM'G^t}$ is also identical with the that of the standard case, where large accuracy improvement is obtained by the adjustment. These results may seem curious, since the accuracy of cross-sections are improved, while there are no alterations in the posterior **E-C** values. The answer can be found from Eq.(A.4), that is, the posterior covariance is not concerned with the **E-C** values at all in the adjustment procedure. On the other hand, the cross-sections alterations ***T'-To*** are rather significant, +0.10 for **s1** and -0.10 for **s3**. The contributions of **s1** and **s3** to the posterior **E-C** values cancelled totally, therefore, the **E-C** values are not altered. Note that this large difference of cross-section alterations between **s1** and **s3** stems from very tiny differences of the sensitivity coefficients, +1.01 for **s1** and +0.99 for **s3**. This situation would be very dangerous for the use of adjustment, since physically meaningless difference of the sensitivity coefficients would result in the large movement of the cross-sections.

Fortunately, we can find the anomaly of this Case 5 input from the statistical check. The χ^2_{min} value is 19.98 which extremely exceeds the degree of freedom, 2. Note that we could judge the input should not be adopted in this Case 5 from the χ^2_{min} value, however, it would be difficult to find this kind of abnormal data if we deal with several hundreds of integral parameters in the adjustment. In this case, we might need to apply other screening system such as the comparison of individual **E-C** value with the corresponding total error of the integral parameter, that is, $\boldsymbol{GMG^t + Ve + Vm}$, in Eq.(A.7)

Figure A.5 Simulation of Cross-section Adjustment (Case 5: Effect of Abnormal **E-C** Value)



V. Concluding Remarks

The lessons from this adjustment exercise with a very simple problem are summarized as follows:

a) The accuracy improvement of the integral parameters is caused by the shrinkage of the cross-section covariance, especially by the addition of negative correlation among cross-sections.
b) If a cross-section standard deviation is large, the alteration rate of the cross-section by the adjustment is also large.
c) Positive correlation between cross-sections plays like large standard deviation values of the cross-sections, if the sensitivity coefficients and other integral parameters are consistent.
d) Large sensitivity coefficients work as large standard deviation values of cross-sections, if the prior **E-C** values are consistent with other parameters.
e) Large error values of integral parameters mean that the data have little influence, or less weight, to the adjusted results.
f) If the sensitivity coefficients and the prior **E-C** values are inconsistent with small integral error values, the adjusted results tend to be dangerously fictitious. Some statistical checks would help to eliminate such erroneous data.

References

1. J.B.Dragt, et al.: "Methods of Adjustment and Error Evaluation of Neutron Capture Cross Sections; Application to Fission Product Nuclides", Nuclear Science and Engineering 62, pp.117-129, 1977.
2. D.L.Smith: "Probability, Statistics, and Data Uncertainties in Nuclear Science and Technology", An OECD Nuclear Energy Agency Nuclear Data Committee Series, Volume 4, American Nuclear Society, 1991.