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Cross section adjustment methods based on minimum variance unbiased estimation

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On the basis of the minimum variance approach, the unified formulation for three types of the cross-section adjustment methods has been derived in a straightforward way without assuming the normal distribution. These methods are intended to minimize the variances of the predicted target core parameters, the adjusted cross-section set, and the calculated integral experimental values. The first and the second methods are found to be slightly different from the extended and the conventional cross-section adjustment methods based on the Bayesian approach with the normal distribution assumption, respectively. However, they become equivalent in some cases and results. The third method is a new method, which is necessary from the viewpoint of the symmetry of the formulation. In addition, it is verified by numerical calculations that the derived formulation gives the minimized variances as intended. The derivation procedure proposed in the present paper is potentially applicable to developing more sophisticated cross-section adjustment methods because of the less assumptions on the probability density function.

\textit{Keywords: cross section adjustment; minimum variance unbiased estimation; maximum likelihood estimation; Bayes’ theorem; normal distribution; uncertainty; covariance;}
1. Introduction

The cross-section adjustment methodology has been widely used as a promising design method for an innovative nuclear reactor system such as a fast reactor. It enables one to improve prediction accuracy of the target core parameters by using integral experimental data measured in critical assemblies and experimental/prototype reactor cores. The methodology is now utilized worldwide. For instance, a comprehensive comparison study of the methodology was recently performed in the international framework[1]. Early proposals of the cross-section adjustment methodology were presented in the 1960s (e.g.[2,3]) and the formulations of the methodology were well-established in the 1970s (e.g.,[4,5,6]). In parallel, a lot of application studies were conducted by many authors, and the formulation of the prediction accuracy for the target core parameters was also accomplished in the 1980s (e.g.,[7]). The cross-section adjustment methodology is also expected to be applied to light water reactors because its applications are successful in recent studies (e.g.,[8]).

On the other hand, the bias factor method is one of the design methods, and it has been still enhanced. Several improved bias factor methods that can utilize more than (or equal to) one integral experimental data unlike the conventional method, such as the generalized bias factor method[9] and the extended bias factor method[10], were proposed in the 2000s. Moreover, it was found that the formulation of the extended bias factor method can be unified with that of the extended cross-section adjustment method (EA)[11], which covers that of the conventional cross-section adjustment method (CA) as a special case.

The formulation of EA is derived by the maximum likelihood estimation (MLE) under the assumption that all variables are normally distributed. However, the formulation of the extended bias method is derived without assuming a specific probability density function by the minimum variance approach. This fact implies that the formulations of EA and
CA can be derived without assuming the normal distribution. The equivalency of the Bayesian approach and the least-square technique relating to the adjustment methodology was discussed by many authors (e.g., [12]). Actually, it was pointed out by Muir that the adjustment equations derived from the minimum variance viewpoint are equivalent to those obtained from the maximum likelihood argument [13]. However, in his paper, a detailed comparison of the equations has not been made from the viewpoint of the cross-section adjustment method for reactor design. In addition, since his derivation includes heuristic procedures, it would be difficult to apply them to developing a new adjustment method.

In the present paper, we show that the formulations similar to EA and CA can be derived in a straightforward way based on the minimum variance unbiased estimation (MVUE) without assuming a specific probability density function. Furthermore, we derive another adjustment equation, called regressive cross-section adjustment method (RA), to complete the symmetry of the formulation. These three cross-section adjustment methods based on MVUE are proposed as EA-MVUE, CA-MVUE, and RA-MVUE with a unified formula. Moreover, we show the formulas of the variance-covariance matrixes for the adjusted cross-section set, the target core parameters and the integral experimental parameters, which are necessary for evaluating the design prediction accuracy.

In Section 2, the nomenclatures used in the present paper are defined and the cross-section adjustment formulas based on MLE are briefly reviewed. In Section 3, the assumptions required in the derivation are described. In Section 4, the derivation of the cross-section adjustment formulation based on MVUE is shown. In Section 5, we discuss the derived formulas. In Section 6, numerical verification results are presented. Finally, the concluding remarks are summarized.
2. Preparation

2.1. Nomenclature

Let us begin with defining the nomenclature used in the present paper. In conjunction with the cross-section set that includes a set of \( n_a \) nuclear data to be adjusted, mostly group-wise infinite dilute cross sections, we use five symbols:

- \( T \) is an \( n_a \times 1 \) matrix, \( i.e. \), a column vector, of an arbitrary cross-section set,
- \( T_t \) is an \( n_a \times 1 \) matrix of the true cross-section set,
- \( T_0 \) is an \( n_a \times 1 \) matrix of the unadjusted cross-section set,
- \( \Delta T_0 \) is an \( n_a \times 1 \) matrix of the error of the unadjusted cross-section set, which is defined as
  \[
  \Delta T_0 \equiv T_0 - T_t,
  \]
  \( (1) \)
  and
- \( M \) is an \( n_a \times n_a \) matrix of the variance-covariance matrix of the unadjusted cross-section set, which is defined as
  \[
  M \equiv \text{Var} \left( T_0 \right),
  \]
  \( (2) \)

where \( \text{Var} \left( \cdot \right) \) indicates the variance. More precisely, the variance of an arbitrary column vector \( X \) of random variables is defined as

\[
\text{Var} \left( X \right) \equiv E \left( (X - E(X)) (X - E(X))^T \right),
\]

where \( E \left( \cdot \right) \) denotes the expected value, which is obtained by averaging the random variables over the probability density function. In the above definitions, we basically assume that the infinite dilute cross sections are adjusted. In this case, the error due to the resonance self-shielding calculation should be taken into account in the analysis method error described later.

Next, let us consider \( n^{(1)} \) integral experimental quantities and \( n^{(2)} \) target core parameters, where the superscripts \( (1) \) and \( (2) \) stand for the integral experimental quantities and
the target core parameters, respectively. In conjunction with the calculation values of the integral experimental quantities and the target core parameters, we define six symbols:

- **$R_t^{(i)}$** is an $n^{(i)} \times 1$ matrix of the true integral experimental quantities or the target core parameters,
- **$R_c^{(i)}(T)$** is an $n^{(i)} \times 1$ matrix of the integral experimental quantities or the target core parameters calculated with the cross-section set $T$,
- **$G^{(i)}$** is an $n^{(i)} \times n_a$ matrix of the sensitivity coefficients of the nuclear data with respect to the integral experimental quantities or the target core parameters, which is defined as
  \[
  G^{(i)} \equiv dR_c^{(i)}(T)/dT, \tag{4}
  \]
- **$\Delta m^{(i)}$** is an $n^{(i)} \times 1$ matrix of the analysis method error, which is defined as
  \[
  \Delta m^{(i)} \equiv R_c^{(i)}(T_t) - R_t^{(i)}, \tag{5}
  \]
- **$V_m^{(i)}$** is an $n^{(i)} \times n^{(i)}$ matrix of the variance-covariance matrix with respect to the analysis method error, which is defined as
  \[
  V_m^{(i)} \equiv \text{Var} \left( R_c^{(i)}(T_t) \right), \tag{6}
  \]
  and
- **$V_m^{(12)}$** is an $n^{(1)} \times n^{(2)}$ matrix of the cross-correlation with respect to the analysis method errors between the integral experimental quantities and the target core parameters, which is defined as
  \[
  V_m^{(12)} \equiv \text{Cov} \left( R_c^{(1)}(T_t), R_c^{(2)}(T_t) \right), \tag{7}
  \]
where $\text{Cov} (\cdot)$ represents the cross-covariance, which is also called cross-correlation. More precisely, the cross-covariance of arbitrary column vectors $X$ and $Y$ is defined as
\[
\text{Cov} (X, Y) \equiv E \left( (X - E(X)) (Y - E(Y))^T \right), \tag{8}
\]
Similarly, in conjunction with the measured values of the integral experimental quantities, we define three symbols:

- \( R^{(1)}_e \) is an \( n^{(1)} \times 1 \) matrix of the measured values of the integral experimental quantities,
- \( \Delta e^{(1)} \) is an \( n^{(1)} \times 1 \) matrix of the experimental error of the integral quantities, which is defined as

\[
\Delta e^{(1)} = R^{(1)}_e - R^{(1)}_t, \tag{9}
\]

and

- \( V^{(1)}_e \) is an \( n^{(1)} \times n^{(1)} \) matrix of the variance-covariance matrix with respect to the experimental error,

\[
V^{(1)}_e = \text{Var} \left( R^{(1)}_e \right). \tag{10}
\]

Since the experimental error and the analysis method error are often used as the sum of them, we additionally define it as

\[
V^{(1)}_{e+m} = V^{(1)}_e + V^{(1)}_m. \tag{11}
\]

Here, notice that, when evaluating \( V^{(1)}_e \), we should take into account the errors of input data for analyzing the integral experimental quantities, such as fuel compositions, dimensions, and temperatures. Although the input data are used in the analysis, they are more correlated with the integral experimental quantities than with the analysis methods. On the other hand, we should also consider the errors of input data for analyzing the target core parameters, such as fabrication tolerance, which are not explicitly defined in the present formulation but can be included into \( V^{(2)}_m \).

2.2. Review of the cross-section adjustment methods

Before deriving the formulas of the cross-section adjustment methods based on MVUE, let us review the derivation and the formulation of EA and CA based on MLE (EA-MLE
2.2.1. Review of the formulation of EA-MLE

Based on the Bayes’ theorem, the formulation of EA-MLE is derived by maximizing the likelihood of the target core parameters under the condition that the integral experimental quantities have been observed. In the derivation of EA-MLE, it is assumed that all variables are followed by the normal distribution.

The adjusted cross-section set $T_{EA}^{MLE}$, the variance-covariance matrix of the adjusted cross-section set $M_{EA}^{MLE}$, and the variance of the predicted target core parameters $\text{Var} \left( R_c^{(2)}(T_{EA}^{MLE}) \right)$ for EA-MLE are written as

\begin{equation}
T_{EA}^{MLE} = T_0 + (MG^{(1)T} + G^{(2)}V_m^{(12)T}) \left( G^{(1)T}MG^{(1)} + V_e^{(1)} + V_m^{(1)} \right)^{-1} \left( R_c^{(1)} - R_c^{(1)}(T_0) \right),
\end{equation}

\begin{equation}
M_{EA}^{MLE} = M + (MG^{(1)T} + G^{(2)}V_m^{(12)T}) \left( G^{(1)T}MG^{(1)} + V_e^{(1)} + V_m^{(1)} \right)^{-1} (G^{(2)} + V_m^{(12)})^T
- MG^{(1)T} \left( G^{(1)T}MG^{(1)} + V_e^{(1)} + V_m^{(1)} \right)^{-1} (MG^{(1)T} + G^{(2)} + V_m^{(12)})^T,
\end{equation}

and

\begin{equation}
\text{Var} \left( R_c^{(2)}(T_{EA}^{MLE}) \right) = G^{(2)}M_{EA}^{MLE}G^{(2)} + V_m^{(2)} - K_{EA}V_m^{(12)} - V_m^{(12)T}K_{EA}^T,
\end{equation}

respectively, where

\begin{equation}
K_{EA} = G^{(2)} \left( MG^{(1)T} + G^{(2)} + V_m^{(12)T} \right) \left( G^{(1)T}MG^{(1)} + V_e^{(1)} + V_m^{(1)} \right)^{-1}.
\end{equation}

Here, the superscript $+$ of $G^{(2)+}$ indicates the Moore-Penrose pseudoinverse.

2.2.2. Review of the formulation of CA-MLE

Similarly, the formulation of CA-MLE is derived by maximizing the likelihood of the cross-section set under the same condition. The maximization target, however, differs from EA-MLE. In the derivation of CA-MLE, all variables are assumed to be normally
distributed as well as EA-MLE.

The adjusted cross-section set $T^{MLE}_{CA}$, the variance-covariance matrix of the adjusted cross-section set $M^{MLE}_{CA}$, and the variance of the predicted target core parameters $\text{Var} \left( R^{(2)}_c (T^{MLE}_{CA}) \right)$ for CA-MLE are written as

$$T^{MLE}_{CA} = T_0 + MG^{(1)T} \left( G^{(1)}MG^{(1)T} + V^{(1)}_{e+m} \right)^{-1} \left( R^{(1)}_c - R^{(1)}_c (T_0) \right), \quad (16)$$

$$M^{MLE}_{CA} = M - MG^{(1)T} \left( G^{(1)}MG^{(1)T} + V^{(1)}_{e+m} \right)^{-1} G^{(1)}M, \quad (17)$$

and

$$\text{Var} \left( R^{(2)}_c (T^{MLE}_{CA}) \right) = G^{(2)}M^{MLE}_{CA}G^{(2)} + V^{(2)}_m - K_{CA}V^{(12)}_m - V^{(12)T}_m K_{CA}^T, \quad (18)$$

respectively, where

$$K_{CA} = G^{(2)}MG^{(1)T} \left( G^{(1)}MG^{(1)T} + V^{(1)}_{e+m} \right)^{-1}. \quad (19)$$

Note that the adjusted cross section set for EA-MLE is equivalent to that for CA-MLE if there is no cross-correlation with respect to the analysis method error between the integral experimental quantities and the target core parameters i.e., $V^{(12)}_m = O$. In other words, CA-MLE is a special case of EA-MLE. This fact means that the target core parameters are not taken into account in the stage of the cross-section adjustment in CA-MLE. However, we should consider the cross-correlations between the integral experimental quantities and the target core parameters in the stage of the uncertainty evaluation even in CA-MLE. The terms of $V^{(12)}_m$ in Eq. (18), therefore, still remain.

3. Assumptions

In this section, we describe the assumptions used in the derivation. Note that no assumption on the specific probability density function such as the normal distribution is adopted here.
3.1. Assumption of linearity approximation

Suppose that the variation of the calculation values caused by the cross-section set changes can be evaluated by the first-order approximation as follows:

\[ R_c^{(i)}(T') - R_c^{(i)}(T) \approx G^{(i)}(T' - T) \quad (i = 1, 2). \] (20)

If this approximation is valid, the calculation error component induced by the cross-section set can be written as

\[ R_c^{(i)}(T_0) - R_c^{(i)}(T_t) \approx G^{(i)} \Delta T_0 \quad (i = 1, 2). \] (21)

Furthermore, by using Eq. (5), the total calculation error is denoted with the sum of the analysis method error and the cross-section-induced calculation error:

\[ R_c^{(i)}(T_0) - R_t^{(i)} \approx \Delta m^{(i)} + G^{(i)} \Delta T_0 \quad (i = 1, 2). \] (22)

Finally, by using Eq. (9), the discrepancy between the experimental values and the calculation values is represented as the sum of the experimental error, the analysis method error, and the cross-section-induced error:

\[ R_c^{(1)} - R_c^{(1)}(T_0) \approx \Delta e^{(1)} - \Delta m^{(1)} - G^{(1)} \Delta T_0. \] (23)

3.2. Assumption of unbiased estimate

Although it must be possible to extend our derivation to a certain biased case, we assume here the unbiased estimates for all of the cross-section set, the calculation values of the integral experimental quantities and the target core parameters, and the experimental values. Namely, the expected values of them are equal to the true values. For instance, we have

\[ \text{E} \left( T_0 \right) = T_t, \] (24)

\[ \text{E} \left( R_c^{(i)}(T_t) \right) = R_t^{(i)} \quad (i = 1, 2). \] (25)
and

$$E (R^{(1)}_e) = R^{(1)}_e. \tag{26}$$

Substituting Eqs. (24), (25), and (26) into Eqs. (1), (5), and (9), respectively, we obtain the following equations:

$$E (\Delta T_0) = O_{n_a \times 1}, \tag{27}$$

$$E (\Delta m^{(i)}) = O_{n^{(i)} \times 1} \quad (i = 1, 2), \tag{28}$$

and

$$E (\Delta e^{(1)}) = O_{n^{(1)} \times 1}, \tag{29}$$

where $O_{p \times q}$ stands for the $p \times q$ zero matrix. In case where the size is clear from the context, we simply write $O$ for the zero matrix. This assumption, therefore, means that none of the errors has bias. Moreover, we assume that the errors have finite second moments.

Under these assumptions, by using Eqs. (2), (6), (10), (7), and (3), the covariance matrices are rewritten as

$$M = E \left( (T_0 - E (T_0))(T_0 - E (T_0))^T \right) = E (\Delta T_0 \Delta T_0^T), \tag{30}$$

$$V^{(i)}_m = E \left( (R^{(i)}_c(T_i) - E (R^{(i)}_c(T_i)))(R^{(i)}_c(T_i) - E (R^{(i)}_c(T_i)))^T \right) = E (\Delta m^{(i)} \Delta m^{(i)T}), \tag{31}$$

$$V^{(1)}_e = E \left( (R^{(1)}_e - E (R^{(1)}_e))(R^{(1)}_e - E (R^{(1)}_e))^T \right) = E (\Delta e^{(1)} \Delta e^{(1)T}), \tag{32}$$

and

$$V^{(12)}_m = E \left( (R^{(1)}_c(T_i) - E (R^{(1)}_c(T_i)))(R^{(2)}_c(T_i) - E (R^{(2)}_c(T_i)))^T \right) = E (\Delta m^{(1)} \Delta m^{(2)T}). \tag{33}$$

Here, notice that Eqs. (1), (5), (9), and (24) – (26) have been also used.
### 3.3. Assumption of error independence

It is assumed that the experimental error, the analysis method error, and the cross-section-induced error with respect to the integral experiments are independent of each other. In other words, we can use the following equations:

\[
E(\Delta m^{(1)} \Delta e^{(1)T}) = E(\Delta e^{(1)} \Delta m^{(1)T}) = O_{n^{(1)} \times n^{(1)}},
\]

\[
E\left( (G^{(1)} \Delta T_0) \Delta e^{(1)T} \right) = E\left( \Delta e^{(1)} \left( G^{(1)} \Delta T_0 \right)^T \right) = O_{n^{(1)} \times n^{(1)}},
\]

and

\[
E\left( (G^{(1)} \Delta T_0) \Delta m^{(1)T} \right) = E\left( \Delta m^{(1)} \left( G^{(1)} \Delta T_0 \right)^T \right) = O_{n^{(1)} \times n^{(1)}}.
\]

Similarly, we assume that the analysis method error and the cross-section-induced error with respect to the target core parameters are independent:

\[
E\left( (G^{(2)} \Delta T_0) \Delta m^{(2)T} \right) = E\left( \Delta m^{(2)} \left( G^{(2)} \Delta T_0 \right)^T \right) = O_{n^{(2)} \times n^{(2)}}.
\]

### 3.4. Assumption of linear estimation

Suppose that the estimate of the integral experimental values \( \hat{R}^{(1)} \) can be represented by the linear combination of the differences between the experimental values and calculation values as

\[
\hat{R}^{(1)} = R_c^{(1)}(T_0) + F\left( R_e^{(1)} - R_c^{(1)}(T_0) \right),
\]

where \( F \) is an \( n^{(1)} \times n^{(1)} \) matrix of the linear combination factors.

In addition, it is assumed that the estimate of the integral experimental value can be reproduced by calculating with a certain cross-section set \( \hat{T} \), i.e., \( \hat{R}^{(1)} = R_c^{(1)}(\hat{T}) \).

Thus, we consider \( \hat{T} \) as the estimate of the cross-section set. Then, using Eq. (20), we can transform Eq. (38) into

\[
R_c^{(1)}(\hat{T}) - R_c^{(1)}(T_0) = F\left( R_e^{(1)} - R_c^{(1)}(T_0) \right).
\]
\( \mathbf{G}^{(1)}(\mathbf{T} - \mathbf{T}_0) \approx \mathbf{F}(\mathbf{R}_e^{(1)} - \mathbf{R}_c^{(1)}(\mathbf{T}_0)) \).

By using the Moore-Penrose pseudoinverse, the minimum-norm least-squares solution of the above equation can be written as

\[ \hat{\mathbf{T}} = \mathbf{T}_0 + \mathbf{G}^{(+)} \mathbf{F}(\mathbf{R}_e^{(1)} - \mathbf{R}_c^{(1)}(\mathbf{T}_0)). \]

This equation is considered as the linear model for the cross-section adjustment methodology.

3.5. Assumptions relating to the sensitivity coefficients

Additionally, we adopt some assumptions relating to the sensitivity coefficients. Since the properties of the Moore-Penrose pseudoinverse of the sensitivity matrix depend on the matrix size and the matrix rank, it is necessary to specify them precisely.

3.5.1. Relation of the number of data

In conjunction with the size of the sensitivity matrixes \( \mathbf{G}^{(i)} \), we basically suppose that

\[ n_a > n^{(1)}. \]

This supposition is reasonable because the number of adjusted cross sections becomes larger than the number of integral experimental quantities in a typical application. In other words, we assume the condition of the ill-posed problem. Meanwhile, we should utilize a sufficient number of integral experimental quantities, which is at least larger than the number of target core parameters. That is, we assume that

\[ n^{(1)} > n^{(2)}. \]
3.5.2. Linear independence of the sensitivity coefficients

Moreover, we assume that \( G^{(i)} \) has full row rank. That is,

\[
\text{rank} \left( G^{(i)} \right) = n^{(i)} \quad (i = 1, 2),
\]

(43)

where \( \text{rank} (\cdot) \) represents the matrix rank. In other words, the sensitivity coefficients are required to be linearly independent. In this case, the following equation is satisfied:

\[
G^{(i)} + G^{(i)} = I_{n^{(i)}} \quad (i = 1, 2),
\]

(44)

where \( I_p \) denotes the \( p \times p \) identity matrix. When the order \( p \) is clear, we simply write \( I \).

Meanwhile, in this case, we should notice that

\[
G^{(i)} + G^{(i)} \neq I_{n^{(i)}} \quad (i = 1, 2).
\]

(45)

In contrast, if we assume the well-posed problem, we will have another condition. In the case of the well-posed problem with the assumption that \( G^{(1)} \) has full column rank, \( i.e., \)

\( n_a < n^{(1)} \) and \( \text{rank} \left( G^{(1)} \right) = n_a \), we need to consider the condition that \( G^{(1)} + G^{(1)} = I_{n_a} \) and \( G^{(1)} G^{(1)} + G^{(1)} \neq I_{n^{(1)}} \).

3.5.3. Assumption of the projection simplification

As mentioned before, \( G^{(1)} + G^{(1)} \neq I_{n_a} \) under the condition of the ill-posed problem. However, \( G^{(1)} + G^{(1)} \) has similar properties to the identity matrix. For instance, the following equation holds by definition:

\[
G^{(1)} G^{(1)} + G^{(1)} = G^{(1)} \quad (i = 1, 2).
\]

(46)

This equation means that we can simply replace \( G^{(1)} + G^{(1)} \) by \( I_{n_a} \) if we ensure premultiplying \( G^{(1)} \) to the result later.

Moreover, \( G^{(1)} + G^{(1)} \) is geometrically interpreted as the orthogonal projection onto the row space of \( G^{(1)} \)[14]. In other words, it is an equivalent transformation of the difference vector of the cross-section set into the most sensitive subspace we are interested in. There-
fore, even if we do not premultiply $G^{(i)}$ later, $G^{(i)} + G^{(i)}$ can be approximated by $I_{n_{u}}$ as far as we are concerned in the integral experimental quantities and/or the target core parameters that have similar sensitivity coefficients to $G^{(i)}$. In the present paper, this replacement is called the “projection simplification,” which is represented as

$$G^{(i)} + G^{(i)} \sim I_{n_{u}} \quad (i = 1, 2).$$ (47)

Here, we use the special equal sign $\sim$ for the projection simplification because it is a particular kind of approximation that is related to $G^{(i)}$. The applicability of the projection simplification will be discussed in Sections 5 and 6. As mentioned later, the projection simplification is utilized to derive the formulas that are equivalent to those of the existing cross-section adjustment methods. In addition, we will show that the projection simplification improves the adjusted cross-section set. However, since it is difficult to understand the physical meaning of the projection simplification, we need to carefully use this assumption. In our derivation, the formulation derived without the projection simplification will be referred as the “rigorous” method. If the projection simplification is once applied, it will be renamed and referred as the “simplified” method.

4. Derivation

4.1. Derivation of the adjusted cross-section set

4.1.1. Derivation of the adjusted cross-section set for EA-MVUE

Let us consider a cross-section adjustment method that minimizes the variance of the calculation values of the target core parameters. We call this method EA-MVUE since it is expected to be equivalent to EA-MLE.

By using Eqs. (20), (5), and (1), the target core parameters calculated by the estimate of the cross-section set $\hat{T}$ are written as

$$R_{c}^{(2)}(\hat{T}) = R_{t}^{(2)} + \left(R_{c}^{(2)}(\hat{T}) - R_{c}^{(2)}(T)\right) + \left(R_{c}^{(2)}(T) - R_{t}^{(2)}(T)\right)$$
\[ R^{(2)}_{c}(\hat{T}) \approx R^{(2)}_{t} + G^{(2)}(\hat{T} - T_{t}) + \Delta m^{(2)} \]
\[ = R^{(2)}_{t} + G^{(2)}(\hat{T} - T_{0}) + G^{(2)}\Delta T_{0} + \Delta m^{(2)}. \]

(48)

Substituting Eq. (40) into Eq. (48) and using Eq. (23), we obtain
\[ R^{(2)}_{c}(\hat{T}) = R^{(2)}_{t} + G^{(2)}G^{(1)} + F(\Delta e^{(1)} - \Delta m^{(1)} - G^{(1)}\Delta T_{0}) + G^{(2)}\Delta T_{0} + \Delta m^{(2)} \]
\[ = R^{(2)}_{t} + (G^{(2)} - G^{(2)}G^{(1)} + FG^{(1)}) \Delta T_{0} \]
\[ + G^{(2)}G^{(1)} + F\Delta e^{(1)} - G^{(2)}G^{(1)} + F\Delta m^{(1)} + \Delta m^{(2)}. \]

(49)

Then, by using Eqs. (30) – (33) and (34) – (37), the variance of the calculation values of the target core parameters is represented as
\[ \text{Var} \left( R^{(2)}_{c}(\hat{T}) \right) = E \left( \left( R^{(2)}_{c}(\hat{T}) - R^{(2)}_{t} \right) \left( R^{(2)}_{c}(\hat{T}) - R^{(2)}_{t} \right)^{T} \right) \]
\[ = (G^{(2)} - G^{(2)}G^{(1)} + FG^{(1)}) E(\Delta T_{0}\Delta T_{0}^{T}) \left( G^{(2)} - G^{(2)}G^{(1)} + FG^{(1)} \right)^{T} \]
\[ + (G^{(2)}G^{(1)} + F) E(\Delta e^{(1)}\Delta e^{(1)T}) \left( G^{(2)}G^{(1)} + F \right)^{T} \]
\[ + (G^{(2)}G^{(1)} + F) E(\Delta m^{(1)}\Delta m^{(1)T}) \left( G^{(2)}G^{(1)} + F \right)^{T} \]
\[ + E(\Delta m^{(2)}\Delta m^{(2)T}) \]
\[ - (G^{(2)}G^{(1)} + F) E(\Delta m^{(1)}\Delta m^{(2)T}) - E(\Delta m^{(2)}\Delta m^{(1)T}) \left( G^{(2)}G^{(1)} + F \right)^{T} \]
\[ = G^{(2)}MG^{(2)T} + G^{(2)}G^{(1)}FG^{(1)}MG^{(1)T}F^{T}G^{(1)T}G^{(2)T} \]
\[ - G^{(2)}MG^{(1)T}F^{T}G^{(1)T}G^{(2)T} - G^{(2)}G^{(1)}FG^{(1)}MG^{(2)T} \]
\[ + G^{(2)}G^{(1)}FV_{e}^{(1)}F^{T}G^{(1)T}G^{(2)T} + G^{(2)}G^{(1)}FV_{m}^{(1)}F^{T}G^{(1)T}G^{(2)T} \]
\[ + V_{m}^{(2)} - G^{(2)}G^{(1)}FV_{m}^{(1)} - V_{m}^{(2)T}F^{T}G^{(1)T}G^{(2)T}. \]

(50)

Here, we have also used the following equation for arbitrary matrixes A and B:
\[ (AB)^{T} = B^{T}A^{T}. \]

(51)

In order to minimize the variance, let us consider the partial derivatives of its trace with
respect to the linear combination factor. Then, we obtain

\[
\frac{\partial}{\partial F} \text{tr} \left( \text{Var} \left( R^{(2)}_c (T) \right) \right) = \frac{\partial}{\partial F} \text{tr} \left( G^{(2)} G^{(1)} + FG^{(1)} M G^{(1)T} F^T G^{(1)+T} G^{(2)T} \right) \\
- \frac{\partial}{\partial F} \text{tr} \left( G^{(2)} M G^{(1)T} F^T G^{(1)+T} G^{(2)} \right) - \frac{\partial}{\partial F} \text{tr} \left( G^{(2)} G^{(1)} + FG^{(1)} M G^{(2)T} \right) \\
+ \frac{\partial}{\partial F} \text{tr} \left( G^{(2)} G^{(1)} + F V_e (1) F^T G^{(1)+T} G^{(2)T} \right) \\
+ \frac{\partial}{\partial F} \text{tr} \left( G^{(2)} G^{(1)} + F V_m (1) F^T G^{(1)+T} G^{(2)T} \right) \\
- \frac{\partial}{\partial F} \text{tr} \left( G^{(2)} G^{(1)} + F V^{(12)} \right) - \frac{\partial}{\partial F} \text{tr} \left( V^{(12)T} F^T G^{(1)+T} G^{(2)T} \right) \\
= 2 G^{(1)+T} G^{(2)T} G^{(2)} G^{(1)} + FG^{(1)} M G^{(1)T} \\
- 2 G^{(1)+T} G^{(2)T} G^{(2)} M G^{(1)T} \\
+ 2 G^{(1)+T} G^{(2)T} G^{(2)} G^{(1)} + F V_e (1) \\
+ 2 G^{(1)+T} G^{(2)T} G^{(2)} G^{(1)} + F V_m (1) \\
- 2 G^{(1)+T} G^{(2)T} V^{(12)T}, \quad (52)
\]

where \( \text{tr} (\cdot) \) denotes the matrix trace, i.e., the sum of the diagonal elements. Here, we have used Eq. (51) and the following equations for arbitrary matrixes \( A \) and \( B \):

\[
\text{tr} (A + B) = \text{tr} (A) + \text{tr} (B), \quad (53)
\]

and

\[
\frac{\partial}{\partial X} (A + B) = \frac{\partial}{\partial X} A + \frac{\partial}{\partial X} B; \quad (54)
\]

and the matrix differential formulas for arbitrary constant matrixes \( A, B, \) and \( C \):

\[
\frac{\partial}{\partial X} \text{tr} (AXB) = A^T B^T, \quad (55)
\]

\[
\frac{\partial}{\partial X} \text{tr} (AX^T B) = BA, \quad (56)
\]

and

\[
\frac{\partial}{\partial X} \text{tr} (AXBX^T C) = A^T C^T XB + CAXB. \quad (57)
\]
In addition, we have used that $G^{(1)}MG^{(1)^T}$, $V_e^{(1)}$, and $V_m^{(1)}$ are symmetric:

\[
(\begin{array}{c}
G^{(1)}MG^{(1)^T} = G^{(1)}MG^{(1)^T}, \\
V_e^{(1)^T} = V_e^{(1)}, \\
\end{array})
\]

(58)

(59)

and

\[
V_m^{(1)^T} = V_m^{(1)}. 
\]

(60)

By setting Eq. (52) to zero, one can determine the factors that minimize the variance. Let $F_{\text{rigorous-EA}}$ represent the minimizing factor such that

\[
(\begin{array}{c}
G^{(1)+T}G^{(2)}G^{(1)+} + F_{\text{rigorous-EA}}G^{(1)}MG^{(1)^T} - G^{(1)+T}G^{(2)}G^{(2)}MG^{(1)^T} \\
+ G^{(1)+T}G^{(2)}G^{(1)+} + F_{\text{rigorous-EA}}V_e^{(1)} \\
+ G^{(1)+T}G^{(2)}G^{(1)+} + F_{\text{rigorous-EA}}V_m^{(1)} - G^{(1)+T}G^{(2)}V^{(12)^T} = 0. \\
\end{array})
\]

(61)

Simplifying for $F_{\text{rigorous-EA}}$ and using Eq. (51), we obtain

\[
(\begin{array}{c}
(G^{(2)}G^{(1)+})^T G^{(2)}G^{(1)+} + F_{\text{rigorous-EA}} \left( G^{(1)}MG^{(1)^T} + V_e^{(1)} \right) \\
= (G^{(2)}G^{(1)+})^T \left( G^{(2)}MG^{(1)^T} + V_m^{(12)^T} \right). \\
\end{array})
\]

(62)

Observe that the variance-covariance matrix $G^{(1)}MG^{(1)^T} + V_{e+m}^{(1)}$ is positive definite, i.e., nonsingular. Then, postmultiplying $(G^{(1)}MG^{(1)^T} + V_{e+m}^{(1)})^{-1}$ to the both sides, we obtain

\[
(\begin{array}{c}
(G^{(2)}G^{(1)+})^T G^{(2)}G^{(1)+} + F_{\text{rigorous-EA}} = (G^{(2)}G^{(1)+})^T \left( G^{(2)}MG^{(1)^T} \\
+ V_m^{(12)^T} \right) \left( G^{(1)}MG^{(1)^T} + V_{e+m}^{(1)} \right)^{-1}. \\
\end{array})
\]

(63)

Observe that rank $(A) = \text{rank} (A^T) = \text{rank} (A^+)$ and that rank $(AB) \leq \min(\text{rank} (A), \text{rank} (B))$ for arbitrary matrices $A$ and $B$, where $\min(\cdot)$ stands for the minimum value. Then, it is shown that rank \(\left( (G^{(2)}G^{(1)+})^T G^{(2)}G^{(1)+} \right) \leq n^{(2)}\). Since $(G^{(2)}G^{(1)+})^T G^{(2)}G^{(1)+}$ is an $n^{(1)} \times n^{(1)}$ matrix, it is singular in the light of Eq. (42). Therefore, we solve Eq. (63) for $F_{\text{rigorous-EA}}$ by utilizing the Moore-Penrose pseudoinverse.
as

\[
F_{\text{rigorous-}EA} = \left( (G^{(2)}G^{(1)+})^T G^{(2)}G^{(1)+} \right)^+ (G^{(2)}G^{(1)+})^T (G^{(2)}MG^{(1)+})^T
+ V_{m(12)T} \right) \left( G^{(1)+}MG^{(1)+} + V_{e+m(1)} \right)^{-1}.
\]  

(64)

Since \((A^TA)^+ = A^+ (A^T)^+ \) and \((A^T)^+ = (A^+)^T \) for an arbitrary matrix \(A\), we can reduce the first half of the above equation to

\[
\left( (G^{(2)}G^{(1)+})^T G^{(2)}G^{(1)+} \right)^+ (G^{(2)}G^{(1)+})^T
= (G^{(2)}G^{(1)+})^+ \left( (G^{(2)}G^{(1)+})^T \right)^+ (G^{(2)}G^{(1)+})^T
= (G^{(2)}G^{(1)+})^+ \left( (G^{(2)}G^{(1)+})^+ \right)^T (G^{(2)}G^{(1)+})^T
= (G^{(2)}G^{(1)+})^+ \left( (G^{(2)}G^{(1)+})^+ \right)^T (G^{(2)}G^{(1)+})^+
= (G^{(2)}G^{(1)+})^+.
\]  

(65)

Here, we have used Eq. (51). In addition, notice that \((AA^+)^T = AA^+ \) and \(A^+AA^+ = A^+ \) for any matrix \(A\) by definition. Thus, we obtain

\[
F_{\text{rigorous-}EA} = (G^{(2)}G^{(1)+})^+ (G^{(2)}MG^{(1)+} + V_{m(12)T}) \left( G^{(1)+}MG^{(1)+} + V_{e+m(1)} \right)^{-1}.
\]  

(66)

Substituting Eq. (66) into Eq. (40), we obtain the adjusted cross-section set for the rigorous EA-MVUE:

\[
T_{\text{rigorous-}EA}^{\text{MVUE}} = T_0 + G^{(1)+} (G^{(2)}G^{(1)+})^+ (G^{(2)}MG^{(1)+})^T
+ V_{m(12)T} \right) \left( G^{(1)+}MG^{(1)+} + V_{e+m(1)} \right)^{-1} (R^{(1)} - R^{(1)}(T_0)).
\]  

(67)

Moreover, applying the projection simplification of Eq. (47), we can further reduce the above equation. Since \((AB)^+ = (A^+ AB)^+ (ABB^+)^+ \) for arbitrary matrixes \(A \) and \(B\), we obtain

\[
(G^{(2)}G^{(1)+})^+ = (G^{(2)+}G^{(2)}G^{(1)+})^+ (G^{(2)}G^{(1)+}G^{(1)})^+
\]
Here, we have also used that $(A^+)^+ = A$ for any matrix $A$. Thus, we can simplify Eq. (66) as

\[
F_{\text{rigorous-EA}} \approx (G^{(1)}G^{(2)} + (G^{(2)}M+V_{m}^{(12)})G^{(1)}T + V_{e+m}^{(1)})^{-1}
\]

\[
\approx G^{(1)}(MG^{(1)}T + G^{(2)} + V_{m}^{(12)})^{-1}
\]

\[
\approx F_{\text{simplified-EA}}.
\] (69)

Note that another minimizing factor $F_{\text{simplified-EA}}$ has been defined here because we have used the projection simplification. Substituting Eq. (69) into Eq. (40) and using the projection simplification again, we arrive at the adjusted cross-section set for the simplified EA-MVUE:

\[
T_{\text{MVUE-EA}}^{\text{simplified-EA}} = T_{0} + G^{(1)}G^{(1)}T
\]

\[
+ (G^{(2)} + V_{m}^{(12)})^{-1}(R_{e}^{(1)} - R_{c}^{(1)}(T_{0}))
\]

\[
\approx T_{\text{MVUE-EA}}^{\text{simplified-EA}}.
\] (70)

The above equation is identical to the adjusted cross-section set for EA-MLE of Eq. (12).

In other words, the following equation is satisfied:

\[
T_{\text{MVUE-EA}}^{\text{simplified-EA}} = T_{\text{ELM-MLE}}^{\text{EA}}.
\] (71)

4.1.2. Derivation of the adjusted cross-section set for CA-MVUE

Since CA-MLE is a special case of EA-MLE as mentioned before, the derivation of EA-MVUE has already covered the derivation of CA-MVUE. However, it is indirect and elusive. In this section, we propose a more straightforward and explanatory derivation.
In order to derive the formulation of CA-MVUE, let us consider a cross-section adjustment method that minimizes the variance of the adjusted cross-section set. By using Eq. (1), the estimate of the cross-section set $\hat{T}$ can be written as

$$\hat{T} = T_t + (\hat{T} - T_0) + \Delta T_0.$$  

(72)

Similarly to the derivation of EA-MVUE, substituting Eq. (40) into Eq. (72) and using Eq. (23), we obtain

$$\hat{T} = T_t + (I - G^{(1)+} FG^{(1)}) \Delta T_0 + G^{(1)+} F\Delta e^{(1)} - G^{(1)+} F\Delta m^{(1)}.$$  

(73)

Then, by using Eqs. (30) – (32), the variance-covariance matrix of the cross-section set is written as

$$\text{Var} \left( \hat{T} \right) = \mathbb{E} \left( (\hat{T} - T_t) (\hat{T} - T_t)^T \right)$$

$$= (I - G^{(1)+} FG^{(1)}) \mathbb{E} \left( \Delta T_0 \Delta T_0^T \right) (I - G^{(1)+} FG^{(1)})^T$$

$$+ (G^{(1)+} F) \mathbb{E} \left( \Delta e^{(1)} \Delta e^{(1)^T} \right) (G^{(1)+} F)^T + (G^{(1)+} F) \mathbb{E} \left( \Delta m^{(1)} \Delta m^{(1)^T} \right) (G^{(1)+} F)^T$$

$$= M + G^{(1)+} FG^{(1)} F G^{(1)+^T} F^T G^{(1)+^T} - 2G^{(1)+} F M G^{(1)+^T} F^T G^{(1)+^T} + G^{(1)+} F V^{(1)} F G^{(1)+^T} F^T G^{(1)+^T} \text{Var} \left( \hat{T} \right)$$

(74)

Here, we have also used Eqs. (34) – (37) and ignored cross-correlations among the cross-section error, the integral experimental error, and the analysis method error.

In order to minimize the variance, let us consider the partial derivatives of its trace with respect to the linear combination factor. Using Eqs. (53) – (60), we obtain

$$\frac{\partial}{\partial F} \text{tr} \left( \text{Var} \left( \hat{T} \right) \right) = \frac{\partial}{\partial F} \text{tr} \left( G^{(1)+} FG^{(1)} F G^{(1)+^T} F^T G^{(1)+^T} \right)$$

$$- \frac{\partial}{\partial F} \text{tr} \left( M G^{(1)+^T} F^T G^{(1)+^T} \right)$$

$$- \frac{\partial}{\partial F} \text{tr} \left( G^{(1)+} FG^{(1)} M \right)$$
\[
+ \frac{\partial}{\partial F} \text{tr} \left( (G^{(1)+T}FV^{(1)}_eF^TG^{(1)+T}) \right) \\
+ \frac{\partial}{\partial F} \text{tr} \left( (G^{(1)+T}FV^{(1)}_mF^TG^{(1)+T}) \right) \\
= 2G^{(1)+T}G^{(1)+T}FG^{(1)}MG^{(1)}T \\
- 2G^{(1)+T}MG^{(1)}T \\
+ 2G^{(1)+T}G^{(1)+T}FV^{(1)}_e \\
+ 2G^{(1)+T}G^{(1)+T}FV^{(1)}_m.
\]

(75)

Let \( F_{CA} \) represent the minimizing factor such that

\[
(G^{(1)+T}G^{(1)+T}F_{CA}G^{(1)}MG^{(1)}T - G^{(1)+T}MG^{(1)}T) \\
+ (G^{(1)+T}G^{(1)+T}F_{CA}V^{(1)}_e + G^{(1)+T}G^{(1)+T}F_{CA}V^{(1)}_m) = 0.
\]

(76)

Simplifying for \( F_{CA} \), we obtain

\[
(G^{(1)+T}G^{(1)+T}) F_{CA} \left( G^{(1)}MG^{(1)}T + V^{(1)}_{e+m} \right) = G^{(1)+T}MG^{(1)}T.
\]

(77)

Observe that \( \text{rank} \left( A^T A \right) = \text{rank} \left( A \right) \) and \( \text{rank} \left( A^+ \right) = \text{rank} \left( A \right) \) for any matrix \( A \). Then, it is shown that \( \text{rank} \left( G^{(1)+T}G^{(1)+T} \right) = n^{(1)}. \) Since \( G^{(1)+T}G^{(1)+T} \) is an \( n^{(1)} \times n^{(1)} \) square matrix, it is nonsingular. Premultiplying \( (G^{(1)+T}G^{(1)+T})^{-1} \) and postmultiplying \( (G^{(1)}MG^{(1)}T + V^{(1)}_{e+m})^{-1} \), we obtain

\[
F_{CA} = (G^{(1)+T}G^{(1)+T})^{-1} G^{(1)+T}MG^{(1)}T \left( G^{(1)}MG^{(1)}T + V^{(1)}_{e+m} \right)^{-1} \\
= G^{(1)}MG^{(1)}T \left( G^{(1)}MG^{(1)}T + V^{(1)}_{e+m} \right)^{-1}.
\]

(78)

Here, we have employed that

\[
(G^{(1)+T}G^{(1)+T})^{-1} G^{(1)+T} = G^{(1)}.
\]

(79)

This equation is proved as follows: Let \( X = (G^{(1)+T}G^{(1)+T})^{-1} G^{(1)+T} \). Then, premultiplying...
and postmultiplying $G^{(1)+}$ to the both sides, we obtain
\[
G^{(1)+}XG^{(1)+} = G^{(1)+} \left( G^{(1)+}\mathbf{T}G^{(1)+} \right)^{-1} \left( G^{(1)+}\mathbf{T}G^{(1)+} \right).
\]
\[
G^{(1)+}XG^{(1)+} = G^{(1)+}.
\]
(80)

Recalling that the Moore-Penrose pseudoinverse is unique, $X$ must be the Moore-Penrose pseudoinverse of $G^{(1)+}$, i.e., $X = (G^{(1)+})^+ = G^{(1)}$.

Note that the projection simplification has not been used yet in the derivation of CA-MVUE. That is why we define only one type of minimizing factor matrix for CA-MVUE. Substituting Eq. (78) into Eq. (40), we obtain the adjusted cross-section set for the rigorous CA-MVUE:
\[
T_{\text{rigorous-CA}}^{\text{MVUE}} = T_0 + G^{(1)+}MG^{(1)}T \left( G^{(1)}MG^{(1)}T + V_{\epsilon+m}^{(1)} \right)^{-1} \left( R_{\epsilon}^{(1)} - R_{\epsilon}^{(1)}(T_0) \right).
\]
(81)

Moreover, using the projection simplification, we arrive at the adjusted cross-section set for the simplified CA-MVUE:
\[
T_{\text{rigorous-CA}}^{\text{MVUE}} \overset{(1)}{=} T_0 + MG^{(1)}T \left( G^{(1)}MG^{(1)}T + V_{\epsilon+m}^{(1)} \right)^{-1} \left( R_{\epsilon}^{(1)} - R_{\epsilon}^{(1)}(T_0) \right)
\]
\[
\equiv T_{\text{simplified-CA}}^{\text{MVUE}}.
\]
(82)

The last equation is identical to the adjusted cross-section set for CA-MLE of Eq. (16). In other words, the following equation is satisfied:
\[
T_{\text{simplified-CA}}^{\text{MVUE}} = T_{\text{CA}}^{\text{MLE}}.
\]
(83)

By the way, since we have not used Eq. (44) in the derivation of CA-MVUE, we may assume the well-posed problem, i.e., $n_a < n^{(1)}$, with the condition that $G^{(1)}$ has full column rank instead of the ill-posed problem, i.e., $n_a > n^{(1)}$, with the condition that $G^{(1)}$ has full row rank. In this case, recalling that $G^{(1)+}G^{(1)} = I_{n_a}$, we can derive Eq. (82) without applying the projection simplification of Eq. (47). Namely, the formulation of the adjusted cross-section set for CA-MVUE becomes exactly the same as that for CA-MLE.
in the case of the well-posed problem.

4.1.3. Derivation of the adjusted cross-section set for RA-MVUE

Now, we have already derived the formulation of EA-MVUE and CA-MVUE. Considering the symmetry of the minimization targets, it is natural to propose another cross-section adjustment method that minimizes the variance of the calculation values of the integral experimental quantities. Compared with EA-MVUE, which is extrapolative and progressive from the viewpoint of the intention of improving the prediction accuracy of target core parameters, the third method is considered as interpolative and regressive. In addition, in the sense of optimizing the prediction accuracy of integral experimental quantities by using themselves, it is recursive and regressive. It is, therefore, proposed as the regressive cross-section adjustment method (RA-MVUE).

In this section, the derivation of RA-MVUE is described. This method may not be very effective as a practical design method because the improvement of calculation accuracy of the integral experimental quantities is not the final purpose. However, it is useful for interpreting the physical meaning of the methodology from the theoretical viewpoint.

Similarly to Eq. (48), by using Eq. (20), (5), and (1), the integral experimental values calculated by the estimate of the cross-section set \( \hat{T} \) are written as

\[
R_c^{(1)}(\hat{T}) = R_t^{(1)} + \left( R_c^{(1)}(\hat{T}) - R_c^{(1)}(T_0) \right) + \left( R_c^{(1)}(T_0) - R_t^{(1)} \right)
\]

\[
\approx R_t^{(1)} + G^{(1)}(\hat{T} - T_0) + \Delta m^{(1)}
\]

\[
= R_t^{(1)} + G^{(1)}(\hat{T} - T_0) + G^{(1)} \Delta T_0 + \Delta m^{(1)}.
\]

Substituting Eq. (40) into Eq. (84) and using Eq. (23), we obtain

\[
R_c^{(1)}(T) = R_t^{(1)} + G^{(1)}G^{(1)} + F \left( \Delta e^{(1)} - \Delta m^{(1)} - G^{(1)} \Delta T_0 \right) + G^{(1)} \Delta T_0 + \Delta m^{(1)}
\]

\[
= R_t^{(1)} + \left( G^{(1)} - FG^{(1)} \right) \Delta T_0 + F \Delta e^{(1)} + (I - F) \Delta m^{(1)}.
\]
Here, we have also used Eq. (44). By using Eqs. (30) – (32) and (34) – (36), the variance of the integral experimental values calculated by the arbitrary cross-section set is represented as

\[
\text{Var} \left( R^{(1)}_c(\hat{T}) \right) = E \left( \left( R^{(1)}_c(\hat{T}) - R^{(1)}_t \right) \left( R^{(1)}_c(\hat{T}) - R^{(1)}_t \right)^T \right)
\]

\[
= \left( G^{(1)} - FG^{(1)} \right) E \left( \Delta T_0 \Delta T_0 \right) \left( G^{(1)} - FG^{(1)} \right)^T
\]

\[
+ FE \left( \Delta e^{(1)} \Delta e^{(1)T} \right) F^T + \left( I - F \right) E \left( \Delta m^{(1)} \Delta m^{(1)T} \right) \left( I - F \right)^T
\]

\[
= G^{(1)}M G^{(1)T} + FG^{(1)}M G^{(1)T} F^T - G^{(1)}M G^{(1)T} F^T - FG^{(1)}M G^{(1)T}
\]

\[
+ F V^{(1)}_e F^T + F V^{(1)}_m F^T + V^{(1)}_m - F V^{(1)}_m - V^{(1)}_m F^T.
\]  

(86)

In order to minimize the variance, let us consider the partial derivatives of its trace with respect to the linear combination factor. Using Eqs. (53) – (60), we obtain

\[
\frac{\partial}{\partial F} \text{tr} \left( \text{Var} \left( R^{(1)}_c(\hat{T}) \right) \right) = \frac{\partial}{\partial F} \text{tr} \left( FG^{(1)}M G^{(1)T} F^T \right)
\]

\[
- \frac{\partial}{\partial F} \text{tr} \left( G^{(1)}M G^{(1)T} F^T \right) - \frac{\partial}{\partial F} \text{tr} \left( FG^{(1)}M G^{(1)T} \right)
\]

\[
+ \frac{\partial}{\partial F} \text{tr} \left( F V^{(1)}_e F^T \right) + \frac{\partial}{\partial F} \text{tr} \left( F V^{(1)}_m F^T \right)
\]

\[
- \frac{\partial}{\partial F} \text{tr} \left( F V^{(1)}_m \right) - \frac{\partial}{\partial F} \text{tr} \left( V^{(1)}_m F^T \right)
\]

\[
= 2 FG^{(1)}M G^{(1)T} - 2 G^{(1)}M G^{(1)T}
\]

\[
+ 2 F V^{(1)}_e + 2 F V^{(1)}_m - 2 V^{(1)}_m.
\]  

(87)

Let \( F_{RA} \) represent the minimizing factor such that

\[
F_{RA}G^{(1)}M G^{(1)T} - G^{(1)}M G^{(1)T} + F_{RA} V^{(1)}_e + F_{RA} V^{(1)}_m - V^{(1)}_m = 0.
\]  

(88)

Simplifying for \( F_{RA} \) yields

\[
F_{RA} \left( G^{(1)}M G^{(1)T} + V^{(1)}_{e+m} \right) = G^{(1)}M G^{(1)T} + V^{(1)}_m.
\]  

(89)
Postmultiplying \( \left( G^{(1)}MG^{(1)T} + V_{e+m}^{(1)} \right)^{-1} \) to the both sides, we obtain

\[ F_{RA} = \left( G^{(1)}MG^{(1)T} + V_{m}^{(1)} \right) \left( G^{(1)}MG^{(1)T} + V_{e+m}^{(1)} \right)^{-1}. \] (90)

Substituting Eq. (90) into Eq. (40), we obtain the adjusted cross-section set for the rigorous RA-MVUE:

\[ T_{r}^{MVUE} = T_{0} + G^{(1)} + \left( G^{(1)}MG^{(1)T} + V_{m}^{(1)} \right) \left( G^{(1)}MG^{(1)T} + V_{e+m}^{(1)} \right)^{-1} \left( R_{e}^{(1)} - R_{e}^{(1)}(T_{0}) \right). \] (91)

Using Eq. (44) and applying the projection simplification of Eq. (47), we arrived at the adjusted cross-section set for simplified RA-MVUE:

\[ T_{r}^{MVUE} = T_{0} + G^{(1)} + \left( G^{(1)}MG^{(1)T} + V_{m}^{(1)} \right) \left( G^{(1)}MG^{(1)T} + V_{e+m}^{(1)} \right)^{-1} \left( R_{e}^{(1)} - R_{e}^{(1)}(T_{0}) \right) \]

\[ \approx T_{r}^{MVUE} \] (92)

Note that the last equation is equivalent to neither the adjusted cross-section set for EA-MLE of Eq. (12), nor that for CA-MLE of Eq. (16).

4.1.4. Unified formula of the adjusted cross-section set

Since all the formulas of the adjusted cross-section set have the same form, we can rewrite them as

\[ T_{x}^{MVUE} = T_{0} + B_{x}D^{-1} \left( R_{e}^{(1)} - R_{e}^{(1)}(T_{0}) \right) \]

\[ (x = \text{rigorous-EA, simplified-EA, rigorous-CA, simplified-CA, rigorous-RA, simplified-RA}), \] (93)

where

\[ D = G^{(1)}MG^{(1)T} + V_{e+m}^{(1)}, \] (94)
and

\[
B_x = \begin{cases} 
G^{(1)+}(G^{(2)}G^{(1)+})^T(G^{(2)}MG^{(1)+}T + V_m^{(12)+}) & (x = \text{rigorous-EA}) \\
MG^{(1)+}T + G^{(2)+}V_m^{(12)+} & (x = \text{simplified-EA}) \\
G^{(1)+}G^{(1)+}MG^{(1)+}T & (x = \text{rigorous-CA}) \\
MG^{(1)+}T & (x = \text{simplified-CA}) \\
G^{(1)+}(G^{(1)+}MG^{(1)+}T + V_m^{(1)}) & (x = \text{rigorous-RA}) \\
MG^{(1)+}T + G^{(1)+}V_m^{(1)} & (x = \text{simplified-RA}).
\end{cases}
\]  

The minimizing factor matrixes are redefined as

\[
F_x = G^{(1)}B_xD^{-1}
\]  

\((x = \text{rigorous-EA, simplified-EA, rigorous-CA, simplified-CA, rigorous-RA, simplified-RA}).\)  

Note that the above definition satisfies the following equations:

\[
F_{CA} = F_{\text{rigorous-CA}} = F_{\text{simplified-CA}},
\]

\((97)\)

and

\[
F_{RA} = F_{\text{rigorous-RA}} = F_{\text{simplified-RA}}.
\]

\((98)\)

In addition, the matrixes appearing in the formulas of EA-MLE and CA-MLE are similarly defined as

\[
K_x = G^{(2)}B_xD^{-1}
\]  

\((x = \text{rigorous-EA, simplified-EA, rigorous-CA, simplified-CA, rigorous-RA, simplified-RA}).\)  

\((99)\)

These matrixes will be used later.
4.2. Derivation of the variance-covariance matrix of the adjusted cross-section set

Next, let us derive the variance-covariance matrix of the adjusted cross-section set. By using Eqs. (3) and (24), it is written as

\[ M_x^{MVUE} = \text{Var} \left( T_x^{MVUE} \right) = E \left( (T_x^{MVUE} - T_t) (T_x^{MVUE} - T_t)^T \right). \]  

(100)

Using Eqs. (93), (23), and (1), we obtain

\[ T_x^{MVUE} - T_t = \Delta T_0 + B_x D^{-1} (\Delta e^{(1)} - \Delta m^{(1)} - G^{(1)} \Delta T_0) \]

\[ = (I - B_x D^{-1} G^{(1)}) \Delta T_0 + B_x D^{-1} (\Delta e^{(1)} - \Delta m^{(1)}). \]  

(101)

Substituting the above equation into Eq. (100), we obtain

\[ M_x^{MVUE} = (I - B_x D^{-1} G^{(1)}) M (I - B_x D^{-1} G^{(1)})^T + B_x D^{-1} V_{e+m}^{(1)} D^{-1} B_x^T. \]  

(102)

Expanding the first term in the right hand side of the above equation, we arrive at the variance-covariance matrix of the adjusted cross-section set:

\[ M_x^{MVUE} = M + B_x D^{-1} B_x^T - M G^{(1)T} D^{-1} B_x^T - B_x D^{-1} G^{(1)} M \]

\[(x = \text{rigorous-EA, simplified-EA, rigorous-CA, simplified-CA, rigorous-RA, simplified-RA}). \]  

(103)

This equation is the common formulation of the adjusted cross-section set based on MVUE.

Moreover, substituting Eq. (95) into \( B_x^T \) of the second term in the right hand side of Eq. (103), we can confirm that

\[ M_x^{MVUE}^{\text{simplified-EA}} = M_{\text{EA}}^{MLE}, \]  

(104)
and

\[
M_{\text{simplified-CA}}^{MVUE} = M_{CA}^{MLE}. \tag{105}
\]

### 4.3. Derivation of the variance of the predicted target core parameters

By using Eqs. (3) and (25), the variance of the predicted target core parameters is written as

\[
\text{Var} \left(R_c^{(2)}(T_x^{MVUE}) \right) = E \left( \left( R_c^{(2)}(T_x^{MVUE}) - R_t^{(2)} \right) \left( R_c^{(2)}(T_x^{MVUE}) - R_t^{(2)} \right)^T \right). \tag{106}
\]

Introducing Eq. (93) into the following equation given by Eq. (20):

\[
R_c^{(2)}(T_x^{MVUE}) \approx R_c^{(2)}(T_0) + G^{(2)}(T_x^{MVUE} - T_0), \tag{107}
\]

we obtain

\[
R_c^{(2)}(T_x^{MVUE}) = R_c^{(2)}(T_0) + K_x \left( R_c^{(1)} - R_c^{(1)}(T_0) \right), \tag{108}
\]

where \(K_x\) has been already defined in Eq. (99). Using Eqs. (22) and (23), we obtain

\[
R_c^{(2)}(T_x^{MVUE}) = R_t^{(2)} + G^{(2)} \Delta T_0 + \Delta m^{(2)} + K_x \left( \Delta e^{(1)} - \Delta m^{(1)} - G^{(1)} \Delta T_0 \right)
= R_t^{(2)} + \left( G^{(2)} - K_x G^{(1)} \right) \Delta T_0 + K_x \Delta e^{(1)} + \left( \Delta m^{(2)} - K_x \Delta m^{(1)} \right). \tag{109}
\]

Substituting the above equation into Eq. (106), we obtain

\[
\text{Var} \left(R_c^{(2)}(T_x^{MVUE}) \right) = \left( G^{(2)} - K_x G^{(1)} \right) M \left( G^{(2)} - K_x G^{(1)} \right)^T + K_x V_e^{(1)} K_x^T
+ V_m^{(2)} + K_x V_m^{(1)} K_x^T - V_m^{(12)} K_x - K_x^T V_m^{(12)}
= G^{(2)} M G^{(2)} + K_x D K_x^T - G^{(2)} M G^{(1)T} K_x^T - K_x G^{(1)} M G^{(2)} T
+ V_m^{(2)} - K_x V_m^{(12)} - V_m^{(12)} K_x^T. \tag{110}
\]

On the other hand, premultiplying \(G^{(2)}\) and postmultiplying \(G^{(2)T}\) to Eq. (103) yields

\[
G^{(2)} M_x^{MVUE} G^{(2)T} = G^{(2)} M G^{(2)T} + G^{(2)} B_x D^{-1} (D D^{-1}) B_x^T G^{(2)T}
\]
Using Eq. (99), we can further reduce the above equation to

\[ G^{(2)}M^{(1)}_xD^{-1}B_x^TG^{(2)} - G^{(2)}B_xD^{-1}G^{(1)}MG^{(2)}T. \]  

(111)

By simplifying Eq. (110) with the above equation, the variance of the predicted target core parameters is represented as

\[ \text{Var} \left( R^{(2)}_c(T^{MVUE}_x) \right) = G^{(2)}M^{MVUE}_xG^{(2)T} + V^{(2)}_m - K_xV^{(12)}_m - V^{(12)T}K_x^T \]

\[ x = \text{rigorous-EA, simplified-EA, rigorous-CA, simplified-CA, rigorous-RA, simplified-RA}. \]  

(113)

In the light of Eqs. (104) and (105), the above equation is identical to Eqs. (14) and (18). Namely, the following equations are satisfied:

\[ \text{Var} \left( R^{(2)}_c(T^{MVUE}_{\text{simplified-EA}}) \right) = \text{Var} \left( R^{(2)}_c(T^{MLE}_{EA}) \right), \]  

(114)

and

\[ \text{Var} \left( R^{(2)}_c(T^{MVUE}_{\text{simplified-CA}}) \right) = \text{Var} \left( R^{(2)}_c(T^{MLE}_{CA}) \right). \]  

(115)

4.4. Derivation of the variance of the recalculated integral experimental quantities

The variance of the integral experimental values recalculated with the adjusted cross-section set is not important as a design method. However, it is useful to assess the cross-section adjustment results and to compare the performance among the three cross-section adjustment methods.

Here, we summarize the derivation of the variance of the recalculated integral experimental values. It is similar to the derivation of the variance of the predicted target core
parameters, mostly replacing \( G^{(2)}, V^{(12)}_m, \) and \( K_x \) with \( G^{(1)}, V^{(1)}_m, \) and \( F_x. \)

The variance of the recalculated integral experimental is written as

\[
\text{Var} \left( R^{(1)}_c \left( T^{MVUE}_x \right) \right) = E \left( \left( R^{(1)}_c \left( T^{MVUE}_x \right) - R^{(1)}_t \right) \left( R^{(1)}_c \left( T^{MVUE}_x \right) - R^{(1)}_t \right)^T \right). \tag{116}
\]

Introducing Eq. (93) into the following equation:

\[
R^{(1)}_c \left( T^{MVUE}_x \right) \approx R^{(1)}_c \left( T_0 \right) + G^{(1)} \left( T^{MVUE}_x - T_0 \right), \tag{117}
\]

which is given by Eq. (20), and recalling Eq. (96), we obtain

\[
R^{(1)}_c \left( T^{MVUE}_x \right) = R^{(1)}_c \left( T_0 \right) + F_x \left( R^{(1)}_c - R^{(1)}_c \left( T_0 \right) \right). \tag{118}
\]

By using Eqs. (22) and (23), the above equation is rewritten as

\[
R^{(1)}_c \left( T^{MVUE}_x \right) = R^{(1)}_t + \Delta m^{(1)} + G^{(1)} \Delta T_0 + F_x \left( \Delta e^{(1)} - \Delta m^{(1)} - G^{(1)} \Delta T_0 \right)
\]

\[
= R^{(1)}_t + \left( G^{(1)} - F_x G^{(1)} \right) \Delta T_0 + F_x \Delta e^{(1)} + \left( \Delta m^{(1)} - F_x \Delta m^{(1)} \right). \tag{119}
\]

Substituting the above equation into Eq. (116), we obtain

\[
\text{Var} \left( R^{(1)}_c \left( T^{MVUE}_x \right) \right) = \left( G^{(1)} - F_x G^{(1)} \right) M \left( G^{(1)} - F_x G^{(1)} \right)^T + F_x V^{(1)}_m F_x^T
\]

\[
+ V^{(1)}_m + F_x V^{(1)}_m F_x^T - F_x V^{(1)}_m - V^{(1)}_m F_x^T
\]

\[
= G^{(1)} M G^{(1)} + F_x D F_x^T - G^{(1)} M G^{(1)} F_x^T - F_x G^{(1)} M G^{(1)}^T
\]

\[
+ V^{(1)}_m - F_x V^{(1)}_m - V^{(1)}_m F_x^T. \tag{120}
\]

On the other hand, premultiplying \( G^{(1)} \) and postmultiplying \( G^{(1)}^T \) to Eq. (103) yields

\[
G^{(1)} M^{MVUE}_x G^{(1)}^T = G^{(1)} M G^{(1)}^T + F_x D F_x^T - G^{(1)} M G^{(1)} F_x^T - F_x G^{(1)} M G^{(1)}^T. \tag{121}
\]

Thus, the variance of the recalculated integral experimental quantities is represented as

\[
\text{Var} \left( R^{(1)}_c \left( T^{MVUE}_x \right) \right) = G^{(1)} M^{MVUE}_x G^{(1)} + V^{(1)}_m - F_x V^{(1)}_m - V^{(1)}_m F_x^T
\]

\[x = \text{rigorous-EA, simplified-EA, rigorous-CA, simplified-CA, rigorous-RA, simplified-RA}. \tag{122}\]
5. Discussion

In this section, we discuss the derived formulation especially for relating to the projection simplification.

5.1. Cancellation of the projection simplification

In the derivation of the simplified methods, we have used the projection simplification. However, it is canceled out for the predicted core parameters in the simplified EA-MVUE, and the recalculated integral experimental quantities in both the simplified CA-MVUE and the simplified RA-MVUE.

Since rank \( (AB^+) \leq \min(\text{rank}(A), \text{rank}(B)) \) for arbitrary matrixes \( A \) and \( B \), we obtain rank \( (G^{(2)}G^{(1)})^+ \leq n^{(2)} \). Since \( G^{(2)}G^{(1)}^+ \) is an \( n^{(2)} \times n^{(1)} \) matrix, it is possible to have full row rank. Then, by assuming that \( G^{(2)}G^{(1)}^+ (G^{(2)}G^{(1)}^+)^+ = I_{n^{(2)}} \), it is shown by using Eqs. (108), (99), and (44) that the predicted target core parameters of the rigorous EA-MVUE are equivalent to those of the simplified EA-MVUE as follows:

\[
R_c^{(2)}(T_{\text{rigorous-EA}}) = R_c^{(2)}(T_0) + G^{(2)}(G^{(1)} + V_m^{(12)^T}) D^{-1} (R_e^{(1)} - R_c^{(1)}(T_0))
\]

\[
= R_c^{(2)}(T_0) + (G^{(2)}MG^{(1)} + V_m^{(12)^T}) D^{-1} (R_e^{(1)} - R_c^{(1)}(T_0))
\]

\[
= R_c^{(2)}(T_0) + G^{(2)}(MG^{(1)}T + V_m^{(12)^T}) D^{-1} (R_e^{(1)} - R_c^{(1)}(T_0))
\]

\[
= R_c^{(2)}(T_{\text{simplified-EA}}).
\]

This fact is corresponding to that the design values of the target core parameters by the extended cross-section adjustment method, including both of EA-MVUE and EA-MLE, become equivalent to those by the extended bias factor method[10] regardless of the projection simplification.

As for CA-MVUE, using Eqs. (118) and (96), we can confirm that the recalculated integral experimental quantities of the rigorous CA-MVUE are equivalent to those of the
simplified CA-MVUE as follows:

\[
\mathbf{R}_c^{(1)}(\mathbf{T}_{\text{rigorous-CA}}) = \mathbf{R}_c^{(1)}(\mathbf{T}_0) + \left( \mathbf{G}^{(1)} \mathbf{G}^{(1)+} \left( \mathbf{G}^{(1)+} \mathbf{G}^{(1)+} \right)^{-1} \right) \mathbf{M} \left( \mathbf{G}^{(1)} \mathbf{D}^{1} - \mathbf{R}_c^{(1)} - \mathbf{R}_c^{(1)}(\mathbf{T}_0) \right)
\]

\[
= \mathbf{R}_c^{(1)}(\mathbf{T}_0) + \left( \mathbf{G}^{(1)} \mathbf{G}^{(1)+} \right) \mathbf{M} \left( \mathbf{D}^{1} - \mathbf{R}_c^{(1)} - \mathbf{R}_c^{(1)}(\mathbf{T}_0) \right)
\]

\[
= \mathbf{R}_c^{(1)}(\mathbf{T}_0) + \left( \mathbf{G}^{(1)} \left( \mathbf{M} \mathbf{D}^{1} \right) - \mathbf{R}_c^{(1)} - \mathbf{R}_c^{(1)}(\mathbf{T}_0) \right)
\]

\[
= \mathbf{R}_c^{(1)}(\mathbf{T}_{\text{simplified-CA}}).
\]

Here, we have also used Eqs. (79) and (46).

Similarly, it is shown by using Eqs. (118) and (96) that the recalculated integral experimental quantities of the rigorous RA-MVUE are equivalent to those of the simplified RA-MVUE as follows:

\[
\mathbf{R}_c^{(1)}(\mathbf{T}_{\text{rigorous-RA}}) = \mathbf{R}_c^{(1)}(\mathbf{T}_0) + \left( \mathbf{G}^{(1)} \mathbf{G}^{(1)+} \right) \mathbf{M} \left( \mathbf{D}^{1} - \mathbf{R}_c^{(1)} - \mathbf{R}_c^{(1)}(\mathbf{T}_0) \right)
\]

\[
= \mathbf{R}_c^{(1)}(\mathbf{T}_0) + \left( \mathbf{G}^{(1)} \left( \mathbf{M} \mathbf{D}^{1} \right) + \mathbf{V}_m^{(1)} \right) \mathbf{D}^{1} \left( \mathbf{R}_c^{(1)} - \mathbf{R}_c^{(1)}(\mathbf{T}_0) \right)
\]

\[
= \mathbf{R}_c^{(1)}(\mathbf{T}_{\text{simplified-RA}}).
\]

Here we have also used Eq. (46).

### 5.2. Interpretation of the projection simplification

Next, we consider the case in which the projection simplification is not canceled out. Suppose the singular value decomposition of \( \mathbf{G}^{(i)} \) as

\[
\mathbf{G}^{(i)} = \mathbf{U}^{(i)} \mathbf{\Sigma}^{(i)} \mathbf{V}^{(i)T} \quad (i = 1, 2),
\]

where \( \mathbf{\Sigma}^{(i)} \) is an \( n^{(i)} \times n_a \) rectangular diagonal matrix, \( \mathbf{U}^{(i)} \) is an \( n^{(i)} \times n^{(i)} \) orthogonal matrix, and \( \mathbf{V}^{(i)T} \) is an \( n_a \times n_a \) orthogonal matrix. The singular value decomposition of \( \mathbf{G}^{(i)} \) is interpreted as three sequential geometric transformations composed of the rotation by \( \mathbf{V}^{(i)T} \), the scaling by \( \mathbf{\Sigma}^{(i)} \), and the rotation by \( \mathbf{U}^{(i)} \). Here, notice that the scaling matrix
\( \Sigma^{(i)} \) has \( n^{(i)} \) non-zero diagonal elements because \( G^{(i)} \) is assumed to have full row rank. In addition, the rotation matrixes \( U^{(i)} \) and \( V^{(i)} \) satisfy the following equations by definition:

\[
U^{(i)}U^{(i)T} = U^{(i)T}U^{(i)} = I_{n^{(i)}},
\]

and

\[
V^{(i)}V^{(i)T} = V^{(i)T}V^{(i)} = I_{n_a}.
\]

Similarly, by using the singular value decomposition, \( G^{(i)+} \) is written as

\[
G^{(i)+} = U^{(i)} \Sigma^{(i)+} V^{(i)},
\]

where \( \Sigma^{(i)+} \) is the Moore-Penrose pseudoinverse of \( \Sigma^{(i)} \). Note that \( \Sigma^{(i)+} \) is an \( n_a \times n^{(i)} \) rectangular diagonal matrix, which is represented as

\[
\Sigma^{(i)+} = \begin{pmatrix}
\sigma_1^{-1} & 0 & \cdots & 0 \\
0 & \sigma_2^{-1} & \cdots & \vdots \\
\vdots & \ddots & \ddots & \vdots \\
0 & \cdots & 0 & \sigma_{n^{(i)}}^{-1} \\
0 & 0 & \cdots & 0 \\
0 & \ddots & \ddots & \ddots \\
0 & \cdots & 0 & 0
\end{pmatrix},
\]

where \( \sigma_1, \sigma_2, \ldots, \sigma_{n^{(i)}} \) are the diagonal elements of \( \Sigma^{(i)} \). That is,

\[
\Sigma^{(i)} = \begin{pmatrix}
\sigma_1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\
0 & \sigma_2 & \cdots & \vdots & 0 & 0 & \cdots & \vdots \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots & 0 & \sigma_{n^{(i)}} & 0 & \cdots & 0 & 0
\end{pmatrix}.
\]

Using Eqs. (126), (129), (127), (130), and (131), we obtain

\[
G^{(i)+}G^{(i)} = V^{(i)} \Sigma^{(i)+}U^{(i)T}U^{(i)} \Sigma^{(i)} V^{(i)T} = V^{(i)} \Sigma^{(i)+} \Sigma^{(i)} V^{(i)T} = V^{(i)} I_{n_a, n^{(i)}} V^{(i)T};
\]
where
\[
I_{n_a,n(i)} = \begin{pmatrix} I_{n(i)} & O_{n(i) \times (n_a-n(i))} \\ O_{(n_a-n(i)) \times n(i)} & O_{(n_a-n(i)) \times (n_a-n(i))} \end{pmatrix}.
\] (133)

Thus, we can see that \(G^{(i)}+G^{(i)}\) is corresponding to three sequential geometric transformations composed of the rotation by \(V^{(i)\text{T}}\), the scaling by \(I_{n_a,n(i)}\), and the inverse rotation of the initial rotation by \(V^{(i)\text{T}}\). Moreover, by using Eq. (128), the projection simplification is rewritten as
\[
G^{(i)}+G^{(i)} = V^{(i)}I_{n_a,n(i)}V^{(i)\text{T}}
\]
\[
\approx V^{(i)}I_{n_a}V^{(i)\text{T}} = I_{n_a}.
\] (134)

According to the above equation, the projection simplification is interpreted as the replacement of the scaling matrixes in the geometric transformations. Since the replacement of \(I_{n_a,n(i)}\) by \(I_{n_a}\) corresponds to the modification of the scaling factors from 0 to 1, we may say that the projection simplification is an extension or an extrapolation rather than an approximation.

5.3. Comparison of the minimized trace of the adjusted cross-section set

In order to see the effect of the projection simplification, we discuss the minimized trace of the adjusted cross-section set in the rigorous CA-MVUE and the simplified CA-MVUE. For arbitrary matrixes \(A\) and \(B\), we have
\[
\text{tr}(AB) = \text{tr}(BA).
\] (135)

In addition, notice that \(G^{(1)}+G^{(1)}\) is an idempotent and symmetric matrix, \(i.e.,\)
\[(G^{(1)}+G^{(1)})^2 = G^{(1)}+G^{(1)}\text{ and } (G^{(1)}+G^{(1)})^\text{T} = G^{(1)}+G^{(1)}.\]

Then, using Eqs. (103) and (53), we obtain
\[
\text{tr} \left( M_{\text{rigorous-CA}}^{\text{MVUE}} \right) = \text{tr} (M) + \text{tr} \left( (G^{(1)}+G^{(1)}) (MG^{(1)\text{T}}D^{-1}G^{(1)\text{T}}M) (G^{(1)}+G^{(1)})^\text{T} \right)
\]
\[
- \text{tr} \left( (MG^{(1)\text{T}}D^{-1}G^{(1)\text{T}}M) (G^{(1)}+G^{(1)})^\text{T} \right)
\]
\[- \text{tr} \left( (G^{(1)} + G^{(1)}) (M G^{(1)^T} D^{-1} G^{(1)} M) \right) \]
\[= \text{tr} \left( M \right) + \text{tr} \left( (G^{(1)} + G^{(1)})^2 (M G^{(1)^T} D^{-1} G^{(1)} M) \right) \]
\[- 2 \text{tr} \left( (G^{(1)} + G^{(1)}) (M G^{(1)^T} D^{-1} G^{(1)} M) \right) \]
\[= \text{tr} \left( M \right) - \text{tr} \left( (G^{(1)} + G^{(1)}) (M G^{(1)^T} D^{-1} G^{(1)} M) \right). \quad (136)\]

Furthermore, by using Eqs. (132) and (135), the second term of the right hand side of the above last equation is rewritten as

\[\text{tr} \left( (G^{(1)} + G^{(1)}) (M G^{(1)^T} D^{-1} G^{(1)} M) \right) = \text{tr} \left( V^{(i)} I_{n_a n^{(1)}} V^{(i)^T} (M G^{(1)^T} D^{-1} G^{(1)} M) \right) \]
\[= \text{tr} \left( I_{n_a n^{(1)}} V^{(i)^T} (M G^{(1)^T} D^{-1} G^{(1)} M) V^{(i)} \right) \]
\[= \sum_{i=1}^{n^{(1)}} d_i, \quad (137)\]

where \(d_i\) is the diagonal elements of \(V^{(i)^T} (M G^{(1)^T} D^{-1} G^{(1)} M) V^{(i)}\). Note that \(d_i > 0\) for all \(i = 1, 2, \cdots, n_a\) since this matrix is positive definite.

On the other hand, using Eqs. (17) and (105), we obtain

\[\text{tr} \left( M^{MVUE}_{\text{simplified-CA}} \right) = \text{tr} \left( M \right) - \text{tr} \left( M G^{(1)^T} D^{-1} G^{(1)} M \right). \quad (138)\]

Then, by using Eqs. (128) and (135), the second term of the right hand side of the above equation is rewritten as

\[\text{tr} \left( M G^{(1)^T} D^{-1} G^{(1)} M \right) = \text{tr} \left( V^{(i)} V^{(i)^T} (M G^{(1)^T} D^{-1} G^{(1)} M) \right) \]
\[= \text{tr} \left( V^{(i)^T} (M G^{(1)^T} D^{-1} G^{(1)} M) V^{(i)} \right) \]
\[= \text{tr} \left( I_{n_a} V^{(i)^T} (M G^{(1)^T} D^{-1} G^{(1)} M) V^{(i)} \right) \]
\[= \sum_{i=1}^{n_a} d_i. \quad (139)\]

Comparing Eq. (139) with Eq. (137) in the case where \(n_a > n^{(1)}\), we obtain

\[\text{tr} \left( M^{MVUE}_{\text{rigorous-CA}} \right) > \text{tr} \left( M^{MVUE}_{\text{simplified-CA}} \right) = \text{tr} \left( M^{MLE}_{CA} \right). \quad (140)\]
Thus, we can see that the projection simplification improves the result of the adjusted cross-section set. This fact suggests that we should use the simplified CA-MVUE (or CA-MLE) for practical use. On the other hand, we have shown by Eqs. (71), (83), (104), (105), (114), and (115) that the simplified EA-MVUE and CA-MVUE are identical to EA-MLE and CA-MLE, respectively. Recalling that the formers are derived without assuming the normal distribution by using the projection simplification and the latters are derived with assuming the normal distribution, we may make a conjecture that the projection simplification corresponds to the assumption of the normal distribution. However, we cannot say for sure that the conjecture is true because the projection simplification is used as an \textit{a priori} assumption in our derivation. In order to ensure eliminating the assumption of the normal distribution, we recommend, therefore, to use the rigorous methods as the cross-section adjustment methods based on MVUE. It will be an issue in the future to provide a clearer explanation of the projection simplification.

6. Numerical Verification

In this section, we show numerical calculation results to verify the derived formulation. These calculation results are based on the integral experimental database for the cross-section adjustment set ADJ2010\cite{15,16} but the calculation conditions are simplified to reduce argument.

In this adjustment, the experimental errors of the integral quantities and their correlations are based on the evaluation by experimenters. The analysis method error depends on the analytical method adopted to obtain the calculation value of the integral experiment. When we utilized the continuous-energy Monte Carlo method, the analysis method error is evaluated by the statistical error. When we applied the deterministic method, the analysis method errors and their correlations are estimated by analytical model sensitivity considerations, which are based on the correction factors evaluated by two calculation values
with different analysis models. Details of this methodology are described elsewhere[17].

6.1. Minimum trace

First, we confirm that the intended minimum traces come out of the derived formulation. In this numerical verification, 40 reaction types of 18-group cross sections and delayed neutron fractions for 6 nuclides, \( n_a = 726 \), are adjusted by utilizing the full set of integral experimental quantities in the database, \( n^{(1)} = 488 \). As for the design targets, three core parameters; criticality, central control rod worth, and sodium void reactivity, of a typical 750MWe-class fast breeder reactor core are selected, \( n^{(2)} = 3 \).

The calculation results are shown in Table 1. From this table, it is seen that the trace of the variance-covariance matrix for the rigorous CA-MVUE, EA-MVUE, and RA-MVUE are minimized as intended for the cross-section set, the predicted target core parameter, and the recalculated integral experimental values, respectively. In addition, it is confirmed that the simplified CA-MVUE gives the smaller trace than the rigorous CA-MVUE as shown in Eq. (140).

On the other hand, it is found that the traces of the target core parameters and the adjusted cross-section set for RA-MVUE are much larger than those for EA-MVUE and CA-MVUE. In contrast, the trace of the integral experimental quantities for RA-MVUE is very small. In this case of RA-MVUE, it is considered that overfitting occurs. Since RA-MVUE uses all observations, \( n_a \), the integral experimental quantities, for fitting themselves, it has too many adjusted parameters relative to the number of observations.

[Table 1 about here.]

6.2. Cancellation of the projection simplification

Next, we check if the projection simplification is canceled out as shown in Eqs. (123) – (125). Table 2 shows the recalculated integral experimental quantities by each adjusted
cross-section set. It is seen that the simplified and the rigorous methods have the same result for both CA and RA as expected. On the other hand, we can see the significant differences between the rigorous and the simplified EA-MVUE for all of the criticality, the control rod worth, and the sodium void reactivity. The reason for the differences is considered as the degree of the simplification. As we can see from Eqs. (69), (70), (82) and (92), the derivation of the simplified EA-MVUE requires more projection simplifications than that of the simplified CA-MVUE and RA-MVUE. Furthermore, it is seen from the table that the standard deviations of the rigorous EA-MVUE are larger than those of the simplified EA-MVUE. The difference of the C/E values between the rigorous and the simplified EA-MVUE seems to be consistent with the prediction accuracy, i.e., the standard deviation.

[Table 2 about here.]

Table 3 shows the predicted target core parameters. It is confirmed that the projection simplification is canceled out for the simplified EA-MVUE. From these results, it is found that the adjusted cross-section set of the rigorous EA-MVUE is different from that of the simplified EA-MVUE even though the both methods give the same result on the predicted target core parameters.

[Table 3 about here.]

6.3. Adjusted cross-section set

Last, we compare the adjusted cross section alterations by the rigorous and the simplified CA-MVUE. Figure 1 shows the 18-group cross section alterations of Pu-239 capture together with the other results which are adjusted with respect to 7-group cross sections. Note that the 7-group case becomes the well-posed problem, i.e., \( n_a = 286 < 488 = n^{(1)} \).

It is seen that both the simplified and the rigorous CA-MVUE give almost the same results in the most sensitive and important energy region such as 1keV – 1MeV. However, the
results of the 18-group case differ in the less important energy region such as higher than 1MeV. On the other hand, it is confirmed that the 7-group case gives the same results in all energy ranges. Namely, the rigorous CA-MVUE is equivalent to CA-MLE under the condition of the well-posed problem.

[Figure 1 about here.]

Similarly, the cross section alterations of Pu-241 fission are shown in Fig. 2. Although this reaction is important for core design analysis, the integral experiments sensitive to Pu-241 fission used in the adjustment are less than those sensitive to Pu-239 capture. It is confirmed that the 7-group case provides the same results in all energy ranges as well as the cross-section alterations of Pu-239 capture. However, the results of 18-group case differ even in the important energy region, such as 1keV – 1MeV. While the simplified CA-MVUE gives similar results to those of 7-group case, the rigorous CA-MVUE provides the largely fluctuated results. These results also suggest that we should use the simplified CA-MVUE (or CA-MLE) for practical use.

In summary, we can see that the projection simplification or the assumption of the normal distribution have an important role in the application of the cross-section adjustment methodology.

[Figure 2 about here.]

7. Conclusions

Based on the minimum variance unbiased estimation, three types of cross-section adjustment formulations; the extended cross-section adjustment method (EA-MVUE), the conventional cross-section adjustment method (CA-MVUE), and the regressive cross-section adjustment method (RA-MVUE), have been derived without assuming a specific probability density function such as the normal distribution. EA-MVUE, CA-MVUE, and RA-MVUE minimize the variance of the predicted target core parameters, the variance of
the adjusted cross-section set, and the variance of the recalculated integral experimental values, respectively.

We have derived two variations of the formulas for each method by using the additional assumption of the projection simplification. The simplified EA-MVUE and CA-MVUE, which adopt the projection simplification, are identical to the extended and the conventional cross-section adjustment methods based on the maximum likelihood estimation with the assumption of normal distribution (EA-MLE, CA-MLE), respectively. In contrast, the rigorous EA-MVUE and CA-MVUE, which are derived without the projection simplification, are slightly different from EA-MLE and CA-MLE, respectively. For example, the rigorous EA-MVUE gives the same result as EA-MLE for the predicted target core parameters but not for the adjusted cross-section set. The adjusted cross-section set of the rigorous CA-MVUE differs from that of CA-MLE under the condition of the ill-posed problem, in which the total number of the cross sections to be adjusted is larger than the number of integral experimental quantities. However, the rigorous CA-MVUE becomes equivalent to CA-MLE under the condition of the well-posed problem.

According to the discussion of the minimized trace of CA-MVUE, it is recommended to use the simplified methods for practical use. However, since the projection simplification is not derived deductively from the other assumptions, we should theoretically employ the rigorous methods as the cross-section adjustment methods based on MVUE without the assumption of the normal distribution.

On the other hand, since the derivation procedure described in the present paper is straightforward and requires less assumptions on the probability density function, it offers additional potential to developing an improved methodology, for instance, a cross-section adjustment method that can properly treat biased uncertainties.
Acknowledgment

An author (K.Y.) wishes to express his deep gratitude to Mr. M. Ishikawa of the Japan Atomic Energy Agency for providing useful comments on this manuscript.

References


Table 1 Calculation results of the variance-covariance matrix traces

<table>
<thead>
<tr>
<th></th>
<th>EA-MVUE</th>
<th>CA-MVUE</th>
<th>RA-MVUE</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Target core parameters</strong>¹</td>
<td>rigorous</td>
<td>0.02386*</td>
<td>0.02405</td>
</tr>
<tr>
<td></td>
<td>simplified</td>
<td>0.02386</td>
<td>0.02405</td>
</tr>
<tr>
<td><strong>Adjusted cross-section set</strong>²</td>
<td>rigorous</td>
<td>133.1</td>
<td>4.213*</td>
</tr>
<tr>
<td></td>
<td>simplified</td>
<td>4.195</td>
<td>4.195</td>
</tr>
<tr>
<td><strong>Integral experimental quantities</strong>³</td>
<td>rigorous</td>
<td>1.425</td>
<td>0.9182</td>
</tr>
<tr>
<td></td>
<td>simplified</td>
<td>0.9209</td>
<td>0.9182</td>
</tr>
</tbody>
</table>

1: $\sqrt{\tr(\Var(R_c^{(2)}(T_x)))}$, 2: $\sqrt{\tr(M_x)}$, 3: $\sqrt{\tr(\Var(R_c^{(1)}(T_x)))}$ where $x$ is the method name,

*: the smallest trace among the rigorous EA-MVUE, CA-MVUE, and RA-MVUE.
### Table 2  C/E values of the recalculated integral experimental quantities

<table>
<thead>
<tr>
<th></th>
<th>EA-MVUE</th>
<th>CA-MVUE</th>
<th>RA-MVUE</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>ZPPR-9 KEFF</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>rigorous</td>
<td>1.0022 ± 0.91%*</td>
<td>1.0005 ± 0.06%</td>
<td>1.0005 ± 0.06%</td>
</tr>
<tr>
<td>simplified</td>
<td>1.0009 ± 0.25%</td>
<td>1.0005 ± 0.06%</td>
<td>1.0005 ± 0.06%</td>
</tr>
<tr>
<td><strong>ZPPR-9 CRW</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>rigorous</td>
<td>1.0309 ± 4.42%</td>
<td>0.9904 ± 2.93%</td>
<td>0.9974 ± 0.99%</td>
</tr>
<tr>
<td>simplified</td>
<td>0.9904 ± 2.93%</td>
<td>0.9904 ± 2.93%</td>
<td>0.9974 ± 0.99%</td>
</tr>
<tr>
<td><strong>ZPPR-9 SVR</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>rigorous</td>
<td>1.0511 ± 7.79%</td>
<td>0.9971 ± 4.11%</td>
<td>1.0012 ± 1.59%</td>
</tr>
<tr>
<td>simplified</td>
<td>0.9980 ± 3.89%</td>
<td>0.9971 ± 4.11%</td>
<td>1.0012 ± 1.59%</td>
</tr>
</tbody>
</table>

1: criticality, 2: control rod worth, 3: sodium void reactivity,

*: standard deviation.
Table 3 Correction factors of the predicted target core parameters

<table>
<thead>
<tr>
<th></th>
<th>EA-MVUE</th>
<th>CA-MVUE</th>
<th>RA-MVUE**</th>
</tr>
</thead>
<tbody>
<tr>
<td>750MWe KEFF¹</td>
<td>0.9984 ± 0.15%*</td>
<td>0.9980 ± 0.26%</td>
<td>—</td>
</tr>
<tr>
<td></td>
<td>rigorous</td>
<td>simplified</td>
<td></td>
</tr>
<tr>
<td>750MWe CRW²</td>
<td>0.9690 ± 1.45%</td>
<td>0.9691 ± 1.45%</td>
<td>—</td>
</tr>
<tr>
<td></td>
<td>rigorous</td>
<td>simplified</td>
<td></td>
</tr>
<tr>
<td>750MWe SVR³</td>
<td>0.9689 ± 1.89%</td>
<td>0.9685 ± 1.90%</td>
<td>—</td>
</tr>
<tr>
<td></td>
<td>rigorous</td>
<td>simplified</td>
<td></td>
</tr>
</tbody>
</table>

¹: criticality, 2: control rod worth, 3: sodium void reactivity, 
*: standard deviation, **: no meaningful result available.
Figure Captions

**Figure 1**  Cross section alteration of Pu-239 capture

**Figure 2**  Cross section alteration of Pu-241 fission
Cross section alteration of Pu-239 capture

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Cross Section Adjustment Methods Based on Minimum Variance Unbiased Estimation
Figure 2 Cross section alteration of Pu-241 fission

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Cross Section Adjustment Methods Based on Minimum Variance Unbiased Estimation