Quantification of Integral Data Effectiveness Using the Concept of Active Sub-Space in Nuclear Data Testing

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Several methods based on the concept of the active sub-space are proposed to quantify integral data effectiveness, and they are adopted to existing 32 integral data with multi-group cross section representation. Dimensions of sub-spaces spanned by integral data in a nuclear data space can be quantified with the proposed method using orthogonal projections of each integral data vector to the sub-space. In addition, a method to choose a minimum independent integral data set is proposed, and it is demonstrated that this method can properly choose a wide variety of integral data among a set of dependent integral data.

1 Introduction

In the field of nuclear and radiation engineering, a huge amount of experimental data related to the reactor physics and the radiation shielding have been obtained at various facilities in the world, and some of them have been released to the public as open data to validate numerical tools solving reactor physics and radiation shielding problems. Experimental data which can be utilized to validate nuclear data are referred to as *integral data* in the field of nuclear data engineering, and so many integral data have been accumulated through international projects such as ICSBEP and IRPhEP. Those integral data have been efficiently utilized to test evaluated nuclear data files.

As described above, the number of available integral data has become enormous now, so it is important to choose a proper set of integral data when testing evaluated nuclear data files with them. To do so, dependency among integral data should be carefully examined, so a procedure how to choose proper integral data is desired. We have proposed to adopt the concept of the active sub-space to this problem in our previous study and have tested our method with a set of existing integral data with one-energy group approximation[1] and a set of fictitious integral data with multi-group treatment[2] in the past.

In the present work, we propose a new procedure to quantify independency of a set of integral data and a new method to choose a minimum set of independent integral data among a huge amount of integral data. These methods are adopted to actual integral data with multi-group representation.

2 Theory

2.1 Basic concept of the proposed method

We regard each of nuclear data (ND) is a vector which is orthogonal to other ND vectors, and a *nuclear data space* can be defined from a set of these ND vectors. A sensitivity of integral data with respect to ND is regarded as a vector in the nuclear data space, and a set of sensitivity vectors can span a sub-space, which we call an *integral data space*. Dimension of the integral data space can be defined, and is equal to or smaller than the number of sensitivity vectors. An orthonormal set of basis vectors of the integral data space can be also derived.

If a ND vector exists on the integral data space, this means that this ND can be independently validated with this set of the integral data. On the other hand, if a ND vector does not exist on the integral data space, it is impossible to independently validate this ND with this set of the integral data. In our method, possibility of the independent validation of each ND is quantified by a norm of an orthogonally-projected vector of this ND vector to the integral data space. This is illustrated in **Fig. 1** where a two-dimensional integral data space and a ND vector are presented.

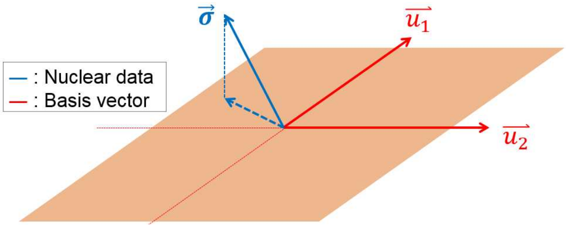

Fig. 1: Relation of an integral data space and a nuclear data vector

2.2 On quantification of integral data space dimension

An orthonormal basis set of an integral data space can be obtained by the singular value decomposition of a sensitivity matrix $\mathbf{S}_{I\times J} = (\mathbf{s}_1\ \mathbf{s}_2\ \cdots\ \mathbf{s}_J)$ where $\mathbf{s}_j$ is a sensitivity vector of the jth integral data and is defined as $\mathbf{s}_j = \left(\frac{dp_j}{d\sigma_1}\ \frac{dp_j}{d\sigma_2}\ \cdots\ \frac{dp_j}{d\sigma_I}\right)^T$, where p_j is a parameter of the jth integral data and σ_i is the ith nuclear data. The superscript T is for vector transposition. The numbers of nuclear data and integral data are denoted to as I and J here. To obtain dimension and an orthonormal basis of the integral data space, the singular value decomposition of $\mathbf{S}$ is carried out as $\mathbf{S} = \mathbf{UDV}^T$ where $\mathbf{U}_{I\times I} = (\mathbf{u}_1\ \mathbf{u}_2\ \cdots\ \mathbf{u}_l\ \cdots \mathbf{u}_I)$ and

$$\mathbf{D}_{I\times J} = \begin{pmatrix} \sigma_1^2 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \sigma_l^2 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}, \tag{1}$$

where l is the dimension and $\mathbf{u}_i$ $(1 \leq i \leq l)$ are orthonormal basis of the integral data space considered here.

Figure 2 shows singular values distributions of several sensitivity matrices obtained in the previous study[1]. Generally, the same number of singular values as the number of integral data is numerically calculated, so we need to determine a threshold value for singular values to separate meaningful components from noise (meaningless) components. As this figure suggests, however, it is very difficult to do this since there is no clear boundary showing drastic change in the behavior.

In the present work, we propose the following procedure to determine the dimension of the integral data space:

1. A set of orthonormal basis vectors is obtained by the singular value decomposition of a sensitivity matrix. Set n=1.

2. Choose n principal basis vectors corresponding to the largest singular values, and construct a n-dimensional sub-space spanned by these n basis vectors.

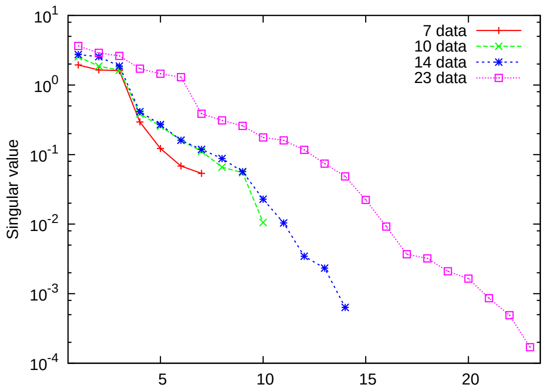

Fig. 2: Example of singular values distributions of sensitivity matrices[1]

3. Each of sensitivity vectors is orthogonally projected to this sub-space, and norms of the projected vectors are calculated. Note that sensitivity vectors are normalized so as to make their norms unity in this step.

4. If the minimum value of the norms obtained at the step 3 is smaller than a criteria, n is increased by one, and a procedure from the step 2 is carried out again. If the minimum norm is larger than this criteria, this procedure is terminated and the dimension of the integral data space is determined as n.

This procedure is based on rather a physical aspect than a mathematical aspect simply setting a criteria on singular values. In the present work, this criteria is set 0.99. Note that obtained results with the proposed method should depend on this parameter setting.

2.3 A method choosing minimum independent data set

There are a huge amount of available integral data, but it is unrealistic to use all of them when testing evaluated nuclear data files. Here we propose a method to choose a minimum independent data set from integral data. The procedure is as follows:

1. The first principal basis vector of the integral data space having the largest singular value is taken, and inner products of this vector and each of sensitivity vectors are calculated. After doing this, a sensitivity vector which gives the largest inner product is chosen as the first integral data.

2. Construct a sub-space spanned by sensitivity vectors of the chosen integral data.

3. Each of non-chosen normalized sensitivity vectors is orthogonally projected to the sub-space constructed at the step 2. If norms of all these projected vectors are larger than a criteria, this procedure is terminated. If not, a sensitivity vector which gives the minimum norm is chosen, and go back to the step 2.

The criteria at the step 3 is arbitrary, and 0.99 is chosen in the present work.

3 Numerical result

The proposed method is adopted to a set of existing integral data shown in **Table 1**. All of these integral data are reactor physics parameters obtained at fast neutron systems, and intetgral data with indices 1 to 16 are for criticality (neutron multiplication factor k), and the others are for fission reaction rate ratio at a core center position. F25, F28, F37 and F23 stand for fission reaction rates of uranium-235, -238, neptunium-237 and uranium-233, respectively. Sensitivities are calculated with 70-group cross section data based on JENDL-4.0. Energy mesh structure of this 70-group cross section data is the same as the JAERI fast set-3, and a whole energy range is divided to 70 with constant lethargy width except the final group. Forward and (generalized) adjoint angular neutron fluxes are calculated by a discrete-ordinate neutron transport solver SNR of the CBZ code system, and sensitivities are calculated with them based on the first-order (generalized) perturbation theory. Sensitivity vectors are normalized so as to make norms of them unity since sensitivities about different reactor physics parameters, k and reaction rate ratio, are considered here.

Table 1: Integral data with their indices

Index	Name	Index	Name
1	Jezebel	17	F23/F25 in Godiva
2	Jezebel-Pu	18	F49/F25 in Godiva
3	Jezebel-233	19	F28/F25 in Jezebel
4	Godiva	20	F37/F25 in Jezebel
5	Flattop-Pu	21	F23/F25 in Jezebel
6	Flattop-U	22	F49/F25 in Jezebel
7	Flattop-233	23	F28/F25 in Jezebel-233
8	Big-ten	24	F37/F25 in Jezebel-233
9	Thor (Pu w Th Ref.)	25	F28/F25 in Flattop-U
10	PMF010 (Pu w NU Ref.)	26	F37/F25 in Flattop-U
11	U3MF002-1 (U-233 w HEU Ref.)	27	F23/F25 in Flattop-U
12	U3MF002-2 (U-233 w HEU Ref.)	28	F49/F25 in Flattop-U
13	U3MF003-1 (U-233 w NU Ref.)	29	F28/F25 in Flattop-Pu
14	U3MF003-2 (U-233 w NU Ref.)	30	F37/F25 in Flattop-Pu
15	F28/F25 in Godiva	31	F28/F25 in Flattop-233
16	F37/F25 in Godiva	32	F37/F25 in Flattop-233

As nuclear data, we consider 8 reactions of (n,f), (n,γ), (n,n), (n,n'), (n,2n), $\bar{\mu}$, $\bar{\nu}$ and χ for the following 10 nuclides: uranium-233, -234, -235, -238, plutonium-239, -240, -241, -242, thorium-232 and neptunium-237. Corresponding indices of these nuclear data are listed in **Table 2**. Since the number of energy groups is 70, the dimension of the nuclear data space considered here is $8\times10\times70$=5,600.

A normalized-singular values distribution of the sensitivity matrix is shown in **Fig. 3**. Two results with and without sensitivity vectors normalization are shown here. The effect of the sensitivity vectors normalization on the singular values distribution is small in the present case.

The principal basis vectors having the largest singular values are shown in **Fig. 4**. On the first basis vector, the first and second highest peaks are observed in (n,f) cross sections of uranium-235 and neptunium-237, respectively, and signs of these components are opposite to each other. This can be considered due to strong contribution of fission reaction rate ratio data of F37/F25. On the second basis vector, the first and second highest peaks are observed in $\bar{\nu}$ and (n,f) cross sections of uranium-233. This can be also considered due to contribution of criticality data of uranium-233-loaded cores. On the third basis vector, the first and second highest peaks are observed in $\bar{\nu}$ and (n,f) cross sections of plutonium-239, and this would be due to contribution of criticality data of plutonium-239-loaded cores.

A dimension of a sub-space spanned by these sensitivities is calculated as 13 with the procedure mentioned above. Since the total number of integral data is 32, it can be concluded that the present data set includes highly-dependent integral data. The result obtained by the proposed method is equivalent with ignoring components whose normalized singular values are less than around 0.075.

Table 2: Nuclear data with their index.

Index	Nuclide	ND	Index	Nuclide	ND	Index	Nuclide	ND
1-	U-233	(n,f)	2241-	Pu-239	(n,f)	4481-	Th-232	(n,f)
71-	U-233	(n,g)	2311-	Pu-239	(n,g)	4551-	Th-232	(n,g)
141-	U-233	(n,n)	2381-	Pu-239	(n,n)	4621-	Th-232	(n,n)
211-	U-233	(n,n')	2451-	Pu-239	(n,n')	4691-	Th-232	(n,n')
281-	U-233	(n,2n)	2521-	Pu-239	(n,2n)	4761-	Th-232	(n,2n)
351-	U-233	$\bar{\mu}$	2591-	Pu-239	$\bar{\mu}$	4831-	Th-232	$\bar{\mu}$
421-	U-233	$\bar{\nu}$	2661-	Pu-239	$\bar{\nu}$	4901-	Th-232	$\bar{\nu}$
491-	U-233	χ	2731-	Pu-239	χ	4971-	Th-232	χ
561-	U-234	(n,f)	2801-	Pu-240	(n,f)	5041-	Np-237	(n,f)
631-	U-234	(n,g)	2871-	Pu-240	(n,g)	5111-	Np-237	(n,g)
701-	U-234	(n,n)	2941-	Pu-240	(n,n)	5181-	Np-237	(n,n)
771-	U-234	(n,n')	3011-	Pu-240	(n,n')	5251-	Np-237	(n,n')
841-	U-234	(n,2n)	3081-	Pu-240	(n,2n)	5321-	Np-237	(n,2n)
911-	U-234	$\bar{\mu}$	3151-	Pu-240	$\bar{\mu}$	5391-	Np-237	$\bar{\mu}$
981-	U-234	$\bar{\nu}$	3221-	Pu-240	$\bar{\nu}$	5461-	Np-237	$\bar{\nu}$
1051-	U-234	χ	3291-	Pu-240	χ	5531-	Np-237	χ
1121-	U-235	(n,f)	3361-	Pu-241	(n,f)			
1191-	U-235	(n,g)	3431-	Pu-241	(n,g)			
1261-	U-235	(n,n)	3501-	Pu-241	(n,n)			
1331-	U-235	(n,n')	3571-	Pu-241	(n,n')			
1401-	U-235	(n,2n)	3641-	Pu-241	(n,2n)			
1471-	U-235	$\bar{\mu}$	3711-	Pu-241	$\bar{\mu}$			
1541-	U-235	$\bar{\nu}$	3781-	Pu-241	$\bar{\nu}$			
1611-	U-235	χ	3851-	Pu-241	χ			
1681-	U-238	(n,f)	3921-	Pu-242	(n,f)			
1751-	U-238	(n,g)	3991-	Pu-242	(n,g)			
1821-	U-238	(n,n)	4061-	Pu-242	(n,n)			
1891-	U-238	(n,n')	4131-	Pu-242	(n,n')			
1961-	U-238	(n,2n)	4201-	Pu-242	(n,2n)			
2031-	U-238	$\bar{\mu}$	4271-	Pu-242	$\bar{\mu}$			
2101-	U-238	$\bar{\nu}$	4231-	Pu-242	$\bar{\nu}$			
2171-	U-238	χ	4411-	Pu-242	χ			

Finally, a minimum set of the independent integral data is also chosen by the proposed method. As a result, the following 18 integral data are chosen. These are presented in the descending order based on their priority: 32, 1, 11, 8, 25, 21, 4, 28, 19, 23, 5, 26, 27, 30, 7, 22, 9 and 2. Detailed information on the first five chosen integral data are provided in **Table 3**. A wide variety of integral data is properly chosen by the proposed algorithm.

4 Conclusion

Several methods based on the concept of the active sub-space have been proposed to quantify integral data effectiveness, and they have been adopted to existing 32 integral data with multi-group cross section representation. Dimensions of sub-spaces spanned by integral data in the nuclear data space can be quantified with the proposed method using orthogonal projections of each integral data vector to the sub-space. In addition, a method to choose a minimum independent integral data set has been proposed, and it has been demonstrated that this method can properly choose

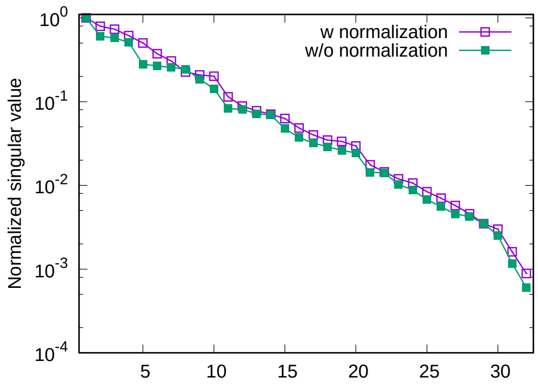

Fig. 3: Singular values distribution of a sensitivity matrix consisting of 32 actual integral data

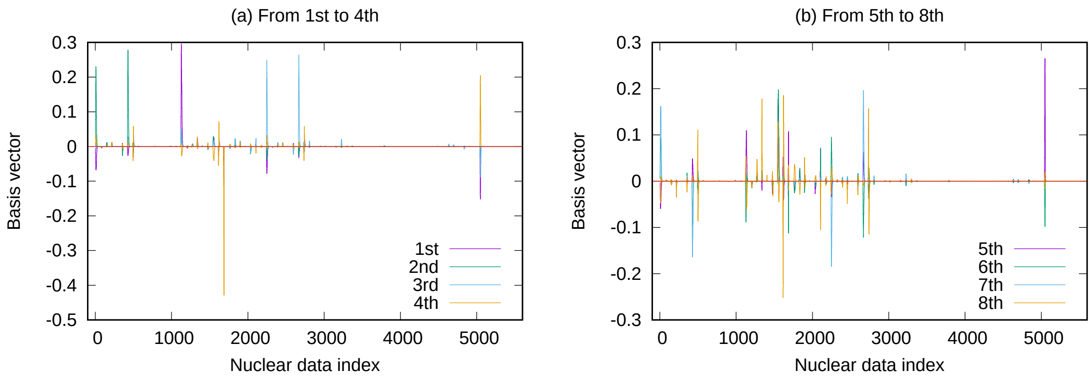

Fig. 4: Principal basis vectors spanning the integral data space of 32 actual integral data

Table 3: Detailed information on the chosen integral data

Priority	Index	Parameter	Fuel material	Reflector material
1	32	F37/F25	U-233	U-238
2	1	k	Pu-239	-
3	11	k	U-233	U-235
4	8	k	U-235, -238	U-238
5	25	F28/F25	U-235	U-238

a wide variety of integral data among a set of dependent integral data.

References

[1] G. Chiba: "Application of active sub-space method to nuclear data integral testing," *the AESJ spring meeting 2016*, (2016).

[2] D. Imazato, G. Chiba: "Quantification of integral data effectiveness by active sub-space," *Proc. of Reactor Physics Asia 2019, RPHA19, Osaka, Japan, Dec. 1-3, 2019*, (2019).