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Application of Multi-Dimensional Principal Component Analysis to Medical Data

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***Abstract*—**Multi-dimensional principal component analysis (PCA) is the extension of the PCA, which is used widely as the dimensionality reduction technique in multivariate data analysis, to handle multi-dimensional data. To calculate the PCA the singular value decomposition (SVD) is commonly employed by the reason of its numerical stability. The multi-dimensional PCA can be calculated by using the higher-order SVD (HOSVD), which is proposed by Lathauwer et al., similarly with the case of ordinary PCA. In this paper, we apply the multi-dimensional PCA to the multi-dimensional medical data including the functional independence measure (FIM) score, and describe the results of experimental analysis.

***Keywords*—** multi-dimensional principal component analysis, higher-order SVD (HOSVD), functional independence measure (FIM), medical data, tensor decomposition

I. Introduction

PRINCIPAL component analysis (PCA) is known as a technique for multivariate data analysis[1], [2]. By using PCA, observed variables are synthesized to several uncorrelated variables, which represent properties of the original multivariate data. Fig. 1 is an example of PCA, by which students' performance (shown in Table I) is analyzed from their scorecard. Students' score on these subjects are plotted in the two-dimensional plane, where the y_1-axis values are language scores and the y_2-axis values are mathematics scores. We show that the synthetic variables can be calculated from the language and the mathematics scores in the figure.

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The 1st principal component, which is named as z_1-axis, is in the direction along which projections have the maximum variance. The 2nd principal component, which is named as z_2-axis, is orthogonal to the first one. Because the z_1-axis values become large as the values both of the y_1-axis and the y_2-axis become large, we see that the z_1-axis expresses these comprehensive characteristics. The z_2-axis also expresses certain comprehensive characteristics. These synthesized axes are called principal axes. The principal components scores are given by projecting students' score onto the principal axes. We can analyze each student's feature by using these principal components scores.

TABLE I
Sample Data for Fig. 1

Student	Score	
	Language y_1	Mathematics y_2
A	80	55
B	70	90
C	90	80
D	55	80
E	40	50
F	50	35

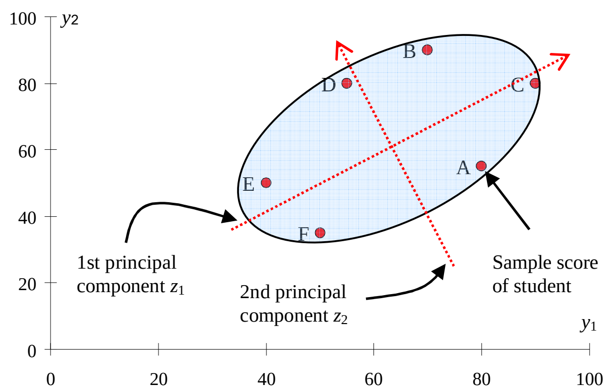

Fig. 1 Conception of the PCA

Multi-dimensional PCA, which is an extension of the ordinary PCA, is proposed to analyze the multi-dimensional sample data. We have studied its application to the analysis of school records, and so on[3], [4]. In this paper, we present the application of multi-dimensional PCA to analyze three-dimensional medical data. As the methods for analysis we adopt two types of extended PCA, namely, the matrix PCA (MPCA) and the third-order tensor PCA (TPCA)[5]. Whereas these methods calculate principal components of multi-dimensional data approximately, the methods for solving optimally these problems by iterative algorithms have been proposed[6], [7]. From the viewpoint of the convenience of calculation, we prefer the MPCA and the TPCA rather than the optimal methods, in this paper.

II. Construction of Multi-dimensional Sample Data

We use medical record data which is furnished by a rehabilitation hospital to perform the feature analysis. The medical record data contains Functional Independence Measure (FIM) values of 9 inpatients whose number of days spent in the hospital is about 3 months. FIM values are scored according to the level of physical assistance required to perform the activities of daily living on a seven-point scale[8], [9]. Each record includes 18 items, of which 13 items are physical items and 5 items are cognitive items. These items are shown in Table II. In the relevant hospital, FIM scores are measured several times during hospitalization to each patient.

TABLE II
Items of Functional Independence Measure

FIM Domain	Item (Subscale) (6)	Item (Detailed Item) (18)
Motor FIM (13)	Self-care	A. Eating, B. Grooming, C. Bathing, D. Dressing upper body, E. Dressing lower body, F. Toileting
	Sphincter control	G. Bladder management, H. Bowel management
	Transfer	I. Bed/chair, J. Toilet, K. Tub/shower
	Locomotion	L. Walk/wheelchair, M. Stairs
Cognitive FIM (5)	Communication	N. Comprehension, O. Expression
	Social cognition	P. Social interaction, Q. Problem solving, R. Memory

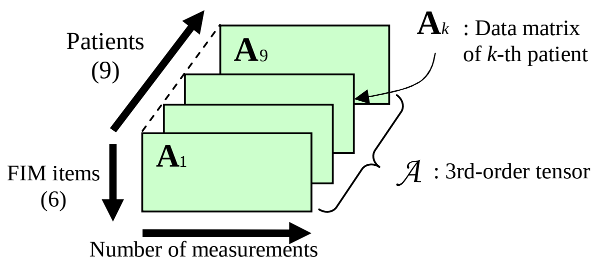

Fig. 2 Structure of 3rd-order tensor medical data

Multi-dimensional data is constructed by piling-up the FIM scores of the patients as shown in Fig. 2. Each FIM score is expressed in a matrix form, where columns are the number of measurements and rows are the measurement items. FIM scores were recorded 8 times for all patients in their hospitalization period. Since the FIM items can be classified into 6 subscales, we defined the FIM value as an average of each FIM value of detailed items that belong to same subscale, and refer simply to these subscales as items, for convenience. Based on the condition above, the multi-dimensional data used here is consisted of 9 matrices which have 6 rows and 8 columns. In this paper, we call each dimension of the multi-dimensional data as a mode, namely in this case, the first mode is the direction of increasing the number of rows, the second mode is the direction of increasing the number of columns, and the third mode is the rest direction. We note that the word "mode" is used here according to precedent papers such as ref. [10].

III. Experimental Analysis by Matrix PCA

A. Calculation Procedure

As described in section I, the principal components that are related to observed variables are calculated by the ordinary PCA. These components are, as we say, 1-mode principal components. On the other hand, by applying the extended PCA, such as MPCA and TPCA, to the *n*-dimensional data we can obtain principal components of multi-modes, that is, 1-mode, 2-mode, ⋯, (*n*-1)-mode.

Since we take up the case of three-dimensional data, or in another word in this section, 3rd-order tensor data, the principal components of two modes are to be obtained by MPCA. In actual experiment, 3rd-order tensor, whose size is $6\times8\times9$, as shown in Fig. 2 is taken up here.

We perform an analysis by the following procedure:

[Step 1]

Calculate the average matrix $\overline{\mathbf{A}}$ as

$$\overline{\mathbf{A}} = (\sum_{k=1}^{9}\mathbf{A}_k)/9\,, \tag{1}$$

where $\mathbf{A}_k$ is a component matrix of the 3rd-order tensor $\mathcal{A}$. Then, using $\overline{\mathbf{A}}$, calculate the standard deviation for each element of $\mathbf{A}_k$ with changing *k* from 1 to 9 as

$$S(i,j) = \sqrt{\frac{1}{9}\sum_{k=1}^{9}\left\{\mathbf{A}_k(i,j) - \overline{\mathbf{A}}(i,j)\right\}^2}\quad , \tag{2}$$

where $S(i,j)$ denotes the (*i*,*j*)th element of standard deviation matrix S, and similarly for the notation $\mathbf{A}_k(i,j)$ and $\overline{\mathbf{A}}(i,j)$.

The 3rd-order tensor $\mathcal{T}$ can be constituted by piling-up the matrix $\mathbf{T}_k$, which is obtained by standardizing each $\mathbf{A}_k$ as

$$\mathbf{T}_k(i,j) = \frac{1}{S(i,j)}\{\mathbf{A}_k(i,j) - \overline{\mathbf{A}}(i,j)\}, \tag{3}$$

for every *i* and *j*.

The matrix $\mathbf{T}_k$ is referred to as the standardized matrix. The 3rd-order tensor $\mathcal{T}$ obviously has the same structure as the original 3rd-order tensor $\mathcal{A}$.

[Step 2]

Decompose the 3rd-order tensor $\mathcal{T}$ by higher-order singular value decomposition (HOSVD) as the following equation[11].

$$\mathcal{T} = \mathcal{C}\times_1\mathbf{U}^{(1)}\times_2\mathbf{U}^{(2)}\times_3\mathbf{U}^{(3)}\,, \tag{4}$$

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where $\mathcal{C}$ is the tensor called core tensor, $\mathbf{U}^{(1)}$, $\mathbf{U}^{(2)}$, and $\mathbf{U}^{(3)}$ are the unitary matrices. These tensor and matrices are combined by *n*-mode products.

The HOSVD is known as an extension of singular value decomposition (SVD), which is the well-known orthogonal decomposition technique of a matrix[12], [13]. Additionally, we subjoin complementary papers [14] and [15] for reference in relation to the convergence and accuracy properties in calculating the HOSVD.

The SVD is very useful technique to calculate coefficients of principal components for the reason of its numerical stability[16], [17]. By applying the SVD to given data matrix, that coefficients are obtained as column vectors of the resultant unitary matrix.

In equation (4), the tensor $\mathcal{C}$ and matrices $\mathbf{U}^{(1)}$, $\mathbf{U}^{(2)}$, and $\mathbf{U}^{(3)}$ correspond to diagonal matrix and unitary matrices that obtained by SVD, respectively. The *n*-mode product is defined as the product of a tensor and a matrix, whose elements are given by summing of products between the elements of a tensor and the elements of *n*-th column vector of a matrix.

Similarly to the case of SVD, the coefficients of *n*-mode principal components are obtained as column vectors of the *n*-th decomposed matrix $\mathbf{U}^{(n)}$, that is, the column vectors of $\mathbf{U}^{(1)}$ and $\mathbf{U}^{(2)}$ denote the coefficients of principal components related to the FIM items and the number of measurements, respectively.

[Step 3]

The principal components score matrix of *k*-th patient can be calculated by multiplying $\mathbf{U}^{(1)^T}$ from the left and $\mathbf{U}^{(2)}$ from the right to the standardized matrix $\mathbf{T}_k$ as

$$\mathbf{Z}_k = \mathbf{U}^{(1)^T}\mathbf{T}_k\mathbf{U}^{(2)}, \tag{5}$$

where $\mathbf{U}^{(1)^T}$ denotes the transpose of $\mathbf{U}^{(1)}$. From the elements of $\mathbf{Z}_k$, we can analyze the feature of *k*-th patient concerning the two modes in combination.

B. Calculation Result

We show the coefficients of the principal components, which are the elements of $\mathbf{U}^{(1)}$ and $\mathbf{U}^{(2)}$, concerning the FIM items (1-mode) and the number of measurements (2-mode) up to the 2nd principal components in Table III, where the abbreviated representation is used as PC for principal component, hereafter. From the table, we see that:

TABLE III
CALCULATED PC COEFFICIENTS OF MPCA

(a) FIM ITEMS

FIM Item (Subscale)	Coefficient	
	1st PC	2nd PC
Self-care	0.42	-0.15
Sphincter control	0.42	-0.19
Transfer	0.42	-0.04
Locomotion	0.36	0.91
Communication	0.41	-0.32
Social cognition	0.41	-0.09
Contribution Rate (%)	92.0	5.6

(b) NUMBER OF MEASUREMENTS

Number	Coefficient	
	1st PC	2nd PC
1	0.34	-0.61
2	0.35	-0.49
3	0.36	-0.16
4	0.36	0.09
5	0.36	0.18
6	0.36	0.23
7	0.36	0.33
8	0.35	0.4
Contribution Rate (%)	96.1	2.6

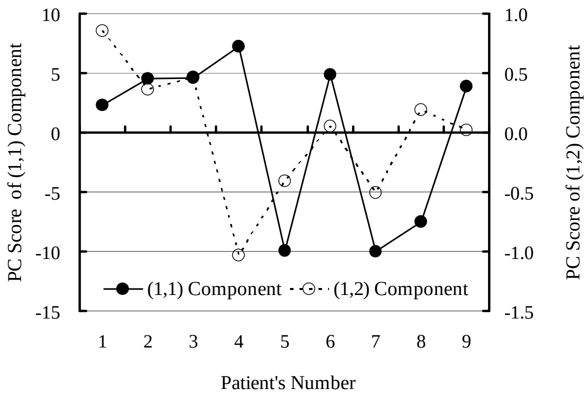

Fig. 3 MPCA scores of (1,1) and (1,2) components.

- The 1st principal components of the both mode express the comprehensive characteristics of each mode.
- The 2nd principal component of the 1-mode expresses the mobility characteristics.
- As for the 2nd principal component of the 2-mode, the rates of weight of the number of measurements are emphasized in the later period of hospitalization.

In Fig. 3, we plot the principal components scores of each patient, which are obtained by the equation (5), in relation to (1,1) and (1,2) components, where the former is the combination of the first components of both modes, and the latter is that of the first component of 1-mode with the second component of 2-mode. From the figure, we see that:

- The (1,1) component expresses the comprehensive characteristics of FIM items over the whole period of hospitalization.
- For this component, the 4th patient has the highest score, on the other hand, the 5th and 7th patients' ones are the lowest scores.

- The (1,2) component expresses the comprehensive characteristics of FIM items in the later period of hospitalization.
- The 1st patient has the highest score in terms of the (1,2) component, although his (1,1) component score is not so high. This fact can be interpreted as saying that the 1st patient is who has a good effect of rehabilitation than other patients.
- In contrast with above patient, although the 4th patient has the highest score in terms of the (1,1) component score, his (1,2) component score is the lowest. The reason of this can be thought that since his FIM score is relatively large in the whole period of hospitalization, there is not much room for improvement for him.
- While the 2nd and 6th patients' (1,1) component scores are approximately equal, the 2nd patient has higher score than the 6th one in terms of the (1,2) component. This means that the improvement of FIM score is significantly higher in the 2nd patient than that in another one.

We show the principal component score of whole patients in Fig. 4, where the horizontal axis is the score of (1,1) component and the vertical axis is that of the (2,2) component. Since the (2,2) component is thought as the property of the improvement on mobility, we see that rehabilitation is effective with respect to mobility for the patients whose score is located in the first quadrant in the figure.

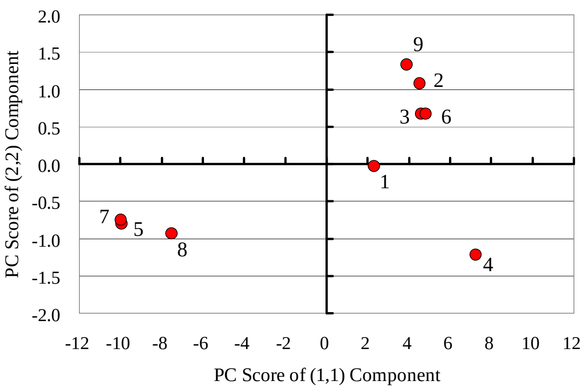

Fig. 4 Correlation chart between (1,1) and (2,2) components of patients, where the number denotes each patient in Fig. 3

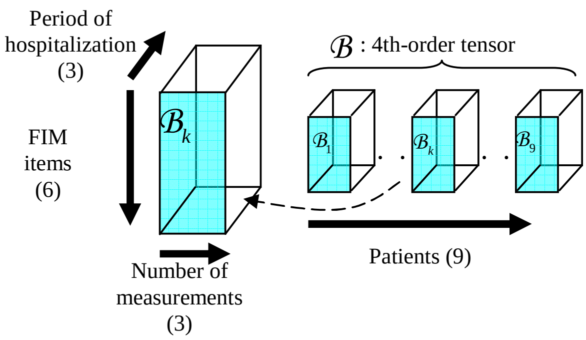

Fig. 5 Structure of 4th-order tensor medical data

IV. Experimental Analysis by Third-order Tensor PCA

A. Calculation Procedure

In this section we also take up the 3rd-order tensor data which mentioned in the previous section with partially changed structure. Here, the numbers of measurements are divided into three groups with regard to the temporal order as the early, middle, and late terms. Then the 3rd-order tensor data of k-th patient is constructed as shown in the left of the Fig. 5, where the 1-mode is the FIM items, 2-mode is the number of measurements in each period, and the 3-mode is the term that divided above. As the right of Fig. 5 shows, the 4th-order tensor data can be constructed by piling-up this tensor for all of the patients. In this way, the 4th-order tensor $\mathcal{B}$ of the size $6\times3\times3\times9$ is obtained to analyze by using TPCA.

In a similar way to the case of MPCA, we can calculate three modes of principal components related to the FIM items, the number of measurements, and the terms in the period. For each patient, principal components scores are obtained as the combination of these three modes by the following procedure:

[Step 1]

The average tensor $\overline{\mathcal{B}}$ can be calculated as

$$\overline{\mathcal{B}} = (\sum_{k=1}^{9} \mathcal{B}_k)/9\,, \tag{6}$$

where $\mathcal{B}_k$ is a component 3rd-order tensor of the 4th-order tensor $\mathcal{B}$. Next, by using $\overline{\mathcal{B}}$, calculate the standard deviation for each element of $\mathcal{B}_k$ with changing k from 1 to 9 as

$$\mathcal{S}(i,j,l) = \sqrt{\frac{1}{9}\sum_{k=1}^{9}\{\mathcal{B}_k(i,j,l) - \overline{\mathcal{B}}(i,j,l)\}^2}\,, \tag{7}$$

where $\mathcal{S}(i,j,l)$ denotes the (i,j,l)th element of standard deviation tensor $\mathcal{S}$, and similarly for the notation $\mathcal{B}_k(i,j,l)$ and $\overline{\mathcal{B}}(i,j,l)$.

Then standardize each $\mathcal{B}_k$ as

$$\mathcal{F}_k(i,j,l) = \frac{1}{\mathcal{S}(i,j,l)}\{\mathcal{B}_k(i,j,l) - \overline{\mathcal{B}}(i,j,l)\}\,, \tag{8}$$

for every i, j, and l.

By piling-up $\mathcal{F}_k$, which is referred to as the standardized tensor, the 4th-order tensor $\mathcal{F}$ is constructed. The structure of the $\mathcal{F}$ is same as the original 4th-order tensor $\mathcal{B}$.

[Step 2]

By applying HOSVD in the same way as the equation (4), the 4th-order tensor $\mathcal{F}$ can be decomposed as follows:

$$\mathcal{F} = \mathcal{D}\times_1 \mathbf{V}^{(1)}\times_2 \mathbf{V}^{(2)}\times_3 \mathbf{V}^{(3)}\times_4 \mathbf{V}^{(4)}\,, \tag{9}$$

where $\mathcal{D}$ is the core tensor, $\mathbf{V}^{(1)}$, $\mathbf{V}^{(2)}$, $\mathbf{V}^{(3)}$, and $\mathbf{V}^{(4)}$ are the unitary matrices. These tensor and matrices are combined by n-mode products. The column vectors of $\mathbf{V}^{(1)}$, $\mathbf{V}^{(2)}$, and $\mathbf{V}^{(3)}$ denote the coefficients of principal components related to the FIM items, the number of measurements, and the terms in the hospitalization, respectively.

[Step 3]

By multiplying the unitary matrices as

$$\mathcal{Z}_k = \mathcal{F}_k \times_1 \mathbf{V}^{(1)^T} \times_2 \mathbf{V}^{(2)^T} \times_3 \mathbf{V}^{(3)^T}, \tag{10}$$

the principal components score tensor of k-th patient is calculated similarly with the equation (5), but the n-mode product notation is used here. The feature of k-th patient can be analyzed by using the elements of $\mathcal{Z}_k$ with regard to the three modes in combination.

B. Calculation Result

Table IV shows the coefficients of the principal components related to three modes that represent the FIM items, the number of measurements, and the terms in the hospitalization period, respectively. From the table, we can see that:

- Every 1st principal component are thought as the comprehended characteristics of the entries of the table for each mode.
- The 2nd principal component of the 1-mode expresses the characteristics related to mobility of the FIM items.
- As for the 2-mode and 3-mode, since the weights of coefficients of the 2nd principal component are emphasized on those of the posterior in each period, these components are thought as the recovery characteristics of the patients.

The principal components scores of the patients are plotted in the Fig. 6, where those scores are calculated as the combination of three modes. The vertical axes show the scores of (1,1,1) and (1,1,2) components individually for the horizontal patient axis. For instance, the (1,1,1) component is a combined characteristics of the 1st principal components of three modes corresponding to sequential order. The (1,1,1) component expresses the comprehensive characteristics of FIM score, and (1,1,2) component does recovery characteristics regarding the whole period in either case. The figure shows an almost similar result with Fig. 3, which is the case of applying the MPCA.

TABLE IV
CALCULATED PRINCIPAL COMPONENTS OF TPCA

(a) FIM ITEMS

FIM Item (Subscale)	Coefficient	
	1st PC	2nd PC
Self-care	0.42	-0.15
Sphincter control	0.42	-0.18
Transfer	0.42	-0.04
Locomotion	0.37	0.9
Communication	0.41	-0.34
Social cognition	0.41	-0.09
Contribution Rate (%)	92.4	5.1

(b) NUMBER OF MEASUREMENTS

Number	Coefficient	
	1st PC	2nd PC
1	0.58	-0.76
2	0.58	0.11
3	0.58	0.64
Contribution Rate (%)	98.8	1.0

(c) TERMS IN HOSPITALIZATION

Term in Hospitalization	Coefficient	
	1st PC	2nd PC
Early term	0.57	-0.81
Middle term	0.58	0.26
Late term	0.58	0.53
Contribution Rate (%)	96.4	3.0

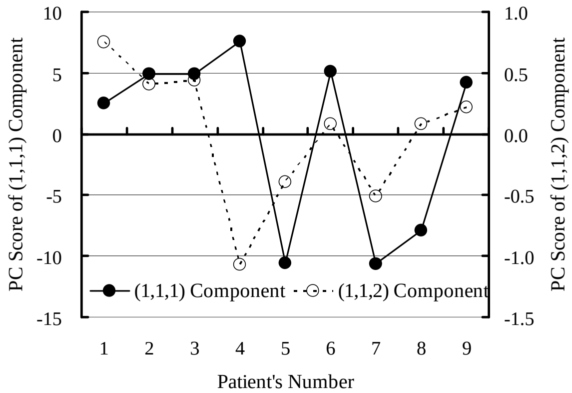

Fig. 6 TPCA scores of (1,1,1) and (1,1,2) components.

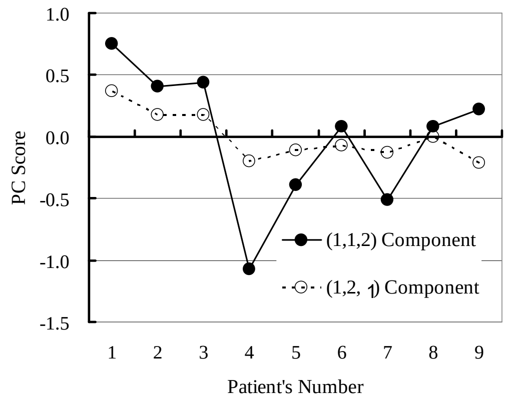

Fig. 7 TPCA scores of (1,1,2) and (1,2,1) components.

In order to perform the further analysis, we plot the principal component scores of (1,1,2) and (1,2,1) for each patient in Fig. 7. Although both components express the recovery characteristics of patients, the former one is associated with the whole period of hospitalization, and the latter with the number of measurements in each term. From the figure, we noticed that though the 9th patient's (1,1,2) score is relatively high, the

(1,2,1) score is the lowest among all patients. As in this way, we could do the detailed analysis regarding to a tendency of recovery for a patient by comparing the scores of the 2-mode and the 3-mode.

V. Conclusion

In this paper, we confirmed the efficiency of the multi-dimensional PCA, such as the MPCA and the TPCA, to analyze the medical data, especially here the FIM score of the hospitalized patients. We discussed the results of 3rd-order tensor and 4th-order tensor data, which were constructed by assuming that:

- The FIM scores of each subscale could be represented by standardizing the measured FIM scores in both of the tensors.
- The 4th-order tensor data could be composed from the set of 3rd-order tensors by dividing the number of measurement into some terms.

Hence, the following problems are remained as future work:

- In order to analyze more precisely the feature of FIM score of the patients, the detailed FIM items shall be used as the variables of 1-mode instead of the subscales.
- Other types of 4th-order tensor data have to be constructed to perform multilateral analysis from views of more variety of combinations of each mode.

Nonetheless, even for the tensor data used here, we could do different types of analysis by changing the ordering of the indices, such as the patients are replaced with the number of measurements, while the FIM items are remained as they were, in Fig. 2. Lastly, we can say that the way of analysis described in this paper could be applicable, with the straightforward modification, to the tensor data of order greater than 4th. We are already proceeding to analyze the 5th-order tensor medical data. The results would be presented in nearly days.

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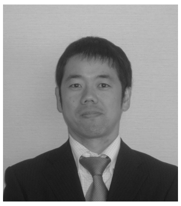

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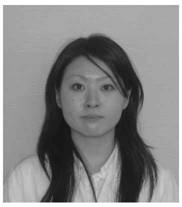
Since 2006, he is working as Chief of the Health Information Management Section, Kumamoto Rehabilitation Hospital.He is a member of the Japan Society of Health Information Management (JHIM).



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