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Clustering for Analysis of Raman Hyperspectral Dental Data

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ABSTRACT

In this research, we presented an effective clustering method based on ICA for the analysis of huge Raman hyperspectral dental data. The hyperspectral dataset captured by HR800 micro Raman spectrometer at UMKC-CRISP(University of Missouri-Kansas City Center for Research on Interfacial Structure and Properties), has 569 local points. Each point has 1,005 hyperspectal dentin data. We compared the clustering effectiveness and the clustering time for the case of using all dataset directly and the cases of using the scores after PCA and ICA. As the result of experiment, the cases of using the scores after PCA and ICA showed, not only more detailed internal dentin information in the aspect of medical analysis, but also about 7~19 times much shorter processing times for clustering. ICA based approach also presented better performance than that of PCA, in terms of the detailed internal information of dentin and the clustering time. Therefore, we could confirm the effectiveness of ICA for the analysis of Raman hyperspectral dental data.

Key words: Hyperspectral Data, Data Clustering, Data Analysis

1. INTRODUCTION

With the development of dental clinic techniques and devices recently, the prevention of dental disease and its treatment which were difficult years ago, have been easier than before. It has contributed to one important part of human well-being. However, we need more academic and practical research and development for better medical service of human being in the future.

According to the statistics, about 70% of all medical illnesses are directly or indirectly caused by human intervention in the dental structures [1]. The most common infectious disease of childhood is dental caries. About 21% of children 6 to 11 have had dental caries in their permanent teeth in the United States [2]. In Korea, recently about 36% of children 6 to 12 have had caries in their permanent teeth [3]. Approximately 15 million people in the United States have had crown and bridge treatment for missing teeth [4].

To solve these dental problems, we need to capture higher quality data related with dental disease and to develop more effective analysis methods. Raman spectrometer is one of important devices to capture hyperspectral dental data and to analyze the symptom of dental disease.

Hyperspectral data means huge captured data across the wide electromagnetic spectrum [5]. Hyperspectral data could be different from multispectral data which has from tens to hundreds of bands, because hyperspectral data has from hundreds to thousands of bands.

The typical research area of hyperspectal data has been the remote sensing area. This research area has received popular attention after the mid

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of 1980s [5]. As an application example of remote sensing hyperspectral data, we can recognize vegetation, soil, lake area etc by using the spectral profile of AVIRIS (Airborne Visible InfraRed Imaging Spectrometer) hyperspectral data [6].

Hyperspectral data has n-dimensional spectral data on a point. These data reflects the characteristic of the point in the spectral domain. The spectral profile of the vegetation area is different from those of urban area and mountain area. Namely, the distribution shape of spectral data can inform us the characteristic of the specific area. In the remote sensing area, we could estimate a certain material by using these spectral profiles.

For huge hyperspectral data analysis, we need effective approach not only to reduce the data volume but also to effectively analyze the data. Principal component analysis (PCA) has been known as one of effective ways to reduce multi-dimensional data sets to lower dimensions. In the relation to the dataset of dental interface, Wang et. el. showed that multivariate approach based on PCA presented more effective analysis than univariate analysis [7].

In the practical dental analysis software tools, such as Hyperview 3.0 in PerkinElemr Inc., Isys 50 in Malvern Instrument and SPF 1.0 in UMKC-CRISP, they partially provide the analysis functions based on PCA, respectively.

In this paper, we found that independent component analysis (ICA) had not applied to the hyprspectral dental data analysis yet. For the first time, we try to apply ICA to effective clustering for Raman hyperspectral data analysis and want to know the effectiveness of ICA in this application. Compared with PCA, ICA has more flexibility about direction than PCA, because it does not need to keep orthogonality. And it also can decide the basic axis by using not only the 2^{nd} order statistic but also the higher-order statistic [8-11].

On the other hand, ICA has medical application areas such as electroencephalography (EEG), magneto encephalography (MEG), electro cardiograph (ECG) and functional magnetic resonance imaging (fMRI) [12-14]. However, most of medical object data are the sampled data in time domain rather than the hyperspectral data.

As hyperspectral data analysis is increasing and multivariate approach using PCA and ICA is more effective one, if we confirm the effectiveness of ICA on the hyperspectral dental data in this research, for the first time, we will apply ICA as the function of the dental analysis. We will practically add it as the function of the dental analysis software tool, SPF 1.0 in UMKC-CRSIP.

2. CLUSTERING FOR HYPERSPECTRAL DATA ANALYSIS

2.1 Clustering system for data analysis

A general block diagram for the hyperspectal data clustering for medical analysis is shown in Fig. 1. Hyperspecteral data is acquired from a hyperspectral input device like Raman spectrometer and stored in a medical hyperspectral database. Before clustering for medical data analysis, we need the preprocessing steps which may contain many procedures such as de-noising, feature extraction, etc. Here, we adopt PCA and ICA as preprocessing steps before the clustering for data analysis. PCA and ICA can not only extract important and specific components but also give data reduction to hyperspectral data.

In general, hyperspectral data is huge, compared with general data, so the clustering over the data directly (which represents the dashed line in Fig. 2) requires a lot of clustering time. This univariate approach usually uses hyperspectral data directly one by one, that is, it uses a single wave number or a peak from each spectrum. It is not enough to analyze hyperspectral data for the complicated region of interest (ROI) [7]. On the other hand, the multivariate approach is to handle whole wave numbers in each spectrum. This approach usually

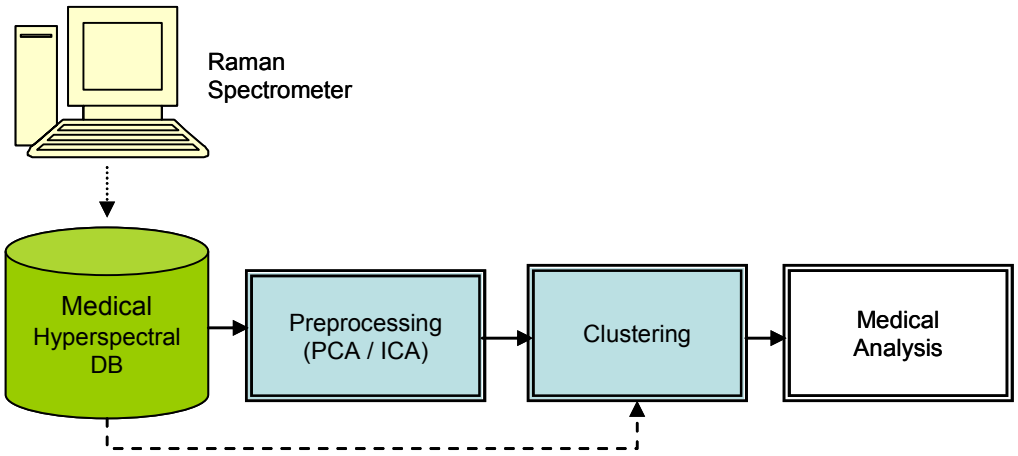


Fig. 1. Clustering system block diagram for hyperspectral data analysis

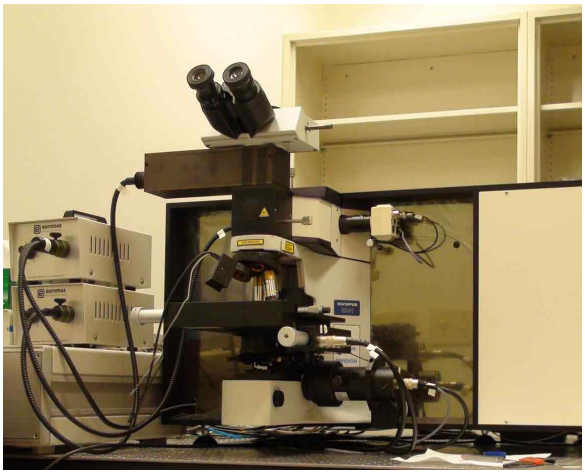


Fig. 2. HR800 micro Raman spectrometer in UMKC-CRISP.

involves the many ways like PCA, clustering methods and the statistical methods.

On the other hand, clustering is one of important steps for medical analysis. It is defined as the process of organizing data into groups whose members are similar in some way. It is a way to find a structure in a collection of unlabeled data, as an unsupervised learning method. In general, the final aim of clustering is related with medical analysis. So, it decides the corresponding grouping for the set of unlabeled data. The best grouping result will be related to the original clustering purpose. Therefore, the users should supply their criterion adequate for the specific applications in order to get the good clustering results for their analysis.

2.2 PCA

Principal component analysis (PCA) is a key statistical technique for multivariate data analysis. It is a vector space transform often used to reduce multidimensional data sets to lower dimensions. PCA is also called discrete Karhunen-Loève Transform (KLT) or Hotelling transform. PCA was invented in 1901 by Karl Pearson. It involves the calculation of the eigenvalue decomposition of a data covariance matrix. PCA is the simplest of the true eigenvector-based multivariate analysis. Often, it can be thought of as revealing the internal structure of the data in a way which best explains the variance in the data. So if a multivariate dataset is visualized as a set of coordinates in a high-dimensional data space, PCA supplies the user with a lower-dimensional picture, a kind of shadow of the object data when viewed from its most informative viewpoint [15].

For large data sets, the common approach to PCA computation is based on the standard NIPALS-PCA algorithm in case of the estimation of the first few components. Non iterative partial least square (NIPALS) algorithm is selected in our research, because it can perform to extract the number of principal components which we desire

to extract from hypersectral data set. The following is its algorithm.

X = data set containing the spectral data in row vectors

t = assumed principal component chosen from X

p = score vector corresponding to the assumption t

E = remnant of the data set

Step 1. initial assumption for the principal component, t_{temp}

Step 2. calculate the corresponding score,

$$p_{temp} = \left(\frac{t^T X}{t^T t} \right)^T$$

Step 3. calculate the normalized score,

$$p = \frac{p_{temp}{}^T}{\left\| p_{temp}{}^T \right\|}$$

Step 4. recalculate the principal component, t using the score, $t = \frac{X p}{p^T p}$

Step 5. if $|t - t_{temp}| < tolernece$, go to Step 6, Otherwise, $t_{temp} = t$ and go to step 2

Step 6. if t is the last component desired to extract, then stop, Otherwise, $E = X - t p^T$, $X = E$ and go to Step 1

First, we initialize, calculate, and normalize the score vector p by using Step 1 to Step 3.

Next, we recalculate the principal component t. with Step 4. Then, in Step 5, if t is within the tolerance, (here we used 0.05 as the tolerance value through the experiment) go to Step 6, otherwise go to Step 2. In Step 6, if t is the last component which we want, the process can stop, but if t is not the last component, we go to Step 1 for calculation of the next component.

2.3 ICA

Independent component analysis (ICA) is a computational method for separating a multivariate signal into additive subcomponents. ICA supposes the mutual statistical independence of the non-Gaussian source signals. It is a special case of blind source separation. When the independence assumption is correct, blind ICA separation of a mixed signal gives very good results. A simple application of ICA is the "cocktail party problem", where the underlying speech signals are separated from a sample data consisting of people talking simultaneously in a room [16].

The statistical method finds the independent components by maximizing the statistical independence of the estimated components. Typical algorithms for ICA use centering, whitening (usually with the eigenvalue decomposition), and dimensionality reduction as preprocessing steps. By using these steps, it can simplify and reduce the complexity of the problem for the actual iterative algorithm. Whitening and dimension reduction can be achieved with principal component analysis or singular value decomposition. There are some algorithms of ICA, including INFOMAX, MISEP, and JADE, and others. Here, we will briefly summarize some typical algorithms.

INFOMAX (Information Maximization) was developed by Bell and Sejnowski in 1995 [17]. But it has some limitations such that it must select the nonlinear function and the function should be fixed. To solve this limitation, in 1998, Almedia proposed MISEP. It adopted the neural network approach to make it adaptive. This can be a generalized INFOMAX [18] which has adaptive characteristic. However, it requires the training of MLP (multilayer neural perceptron). Sometimes its converging is not easy because of the characteristic of input data. JADE (Joint Approximate Diagonalization of Eigen-matrix) was originally developed for digital communication by Cardoso and Souloumiac in 1933 [9]. But it has been used to other applications including medical area like EEG, ECG. JADE has an advantage which can separate specific number of independent components from the input data. It can be a good feature to reduce the computation

load in case of huge dataset like hyperspectral medical data. However, it also has a limitation having certain of number of extraction components depending on the computation platform.

In this research, we select JADE algorithm because we need to extract a specific number of independent components and to reduce the burden of computation on hyperspectral Raman dental data.

The following is the description of JADE-ICA algorithm [19].

X = the observed input data

$\widehat{R}_x$ = corvariance of input data,

$\widehat{W}$= the whitening matrix

$\widehat{Q}_z$ = the 4-th order cumulant

$\hat{B}$= the separating matrix

$\hat{s}$ = the desired separating sources

Step 1. form the corvariance of input data, $\widehat{R}_x$ and compute the whitening matrix, $\widehat{W}$.

Step 2. form the 4^{th} order cumulant $\widehat{Q}_z$ of the whitened process: $\hat{Z} = \widehat{W}$ X

and compute the n most significant eigen pairs $\{\widehat{\lambda}_r, \widehat{M}_r : 1 \le r \le n\}$.

Step 3. jointly diagonalize the n most significant eigen pairs by a unitary matrix $\hat{U}$.

Step 4. estimate of the separating matrix, $\hat{B} = \widehat{W}^{-1}\hat{U}$

Step 5. compute the separating source, $\hat{S} = \hat{B}X$.

First, we do whitening and projection onto single space, $\hat{Z} = \widehat{W}$ X in Step 1. Next, in Step 2, we estimate the cumulant matrix, $\widehat{Q}_z$ and get the most significant eigen pairs. Then, we make joint diagonalization in Step 3. In Step 4, we get the separating matrix, $\hat{B}$ Finally we can have the separating source, $\hat{s}$.

2.4 Clustering Algorithm

In general, clustering algorithm can be classified as exclusive clustering, overlapping clustering, hierarchical clustering, and probabilistic clustering. In exclusive clustering, a datum should exclusively belong to only one cluster, not other clusters. On the other hand, in overlapping clustering, a datum can belong to multiple clusters with different membership values. The membership value of each datum can be represented by fuzzy sets. In hierarchical clustering, each datum initially considered as a cluster. The algorithm hierarchically clusters the dataset by merging two similar nearest cluster. Finally in probabilistic clustering is based on the completely probabilistic approach.

The most used typical clustering algorithms above mentioned are K-means, fuzzy C-means, hierarchical clustering, and mixture of Gaussians. In this research, we use fuzzy C-means algorithm, because it has shown effective results for the analysis of dentin on FTIR data of the adhesive/dentin bond [7].

The following shows fuzzy C-means clustering algorithm.

u_{ij}=membership function of the i^{th} pixel at j^{th} cluster

d_{ij} = distance of the i^{th} pixel at j^{th} cluster

J = dissimilarity function

X = data set containing the spectral data in row vectors

M, N = number of pixels and number of wave number, respectively

n = number of clusters

c = centroid matrix with centroids as row vectors

m = weighting parameter

ε = tolerance for dissimilarity function

Step 1. initialize centroid matrix, c with random data from the data set

Step 2. calculate distance,

$$dij = \sqrt{\sum_{k=1}^{N}(X_{ik} - c_{jk})^2}$$

Step 3. calculate membership function,

$$u_{ij} = \frac{1}{\sum_{k=1}^{n}\left(\frac{d_{ij}}{d_{kj}}\right)^{2/(m-1)}}$$

Step 4. calculate centroid,

$$c_{jk} = \frac{\sum_{i=1}^{M} u_{ij}{}^{m} X_{ik}}{\sum_{i=1}^{M} u_{ij}{}^{m}}$$

Step 5. $J = \sum_{j=1}^{n} J_j = \sum_{i=1}^{M} \sum_{j=1}^{n} u_{ij}{}^{m} d_{ij}{}^{2}$,

Step 6. if $|J' - J| < \varepsilon$ then stop ; other wise $J' - J$, and return to step 2

First, we set centroid matrix and compute the distance between the centroid and the data in Step 1, 2. Next, we get the membership function by using the distance information in Step 3. We compute the updated centroid in Step 4. Then, we calculate the dissimilarity and decide the stop of program running in Step 4, 5 and if not, go to Step 2.

3. EXPERIMENT AND DISCUSSION

3.1 Experimental environment

To capture hyperspectral data for our experiment, HR800 micro Raman spectrometer of HORIBA JOBIN YVON company shown in Figure 2, was used at UMKC-CRSIP. The captured hyperspectral dentain data has 569 local observation points. Each local observation point has 1,005 hyperspectal data over a human premolar with disease.

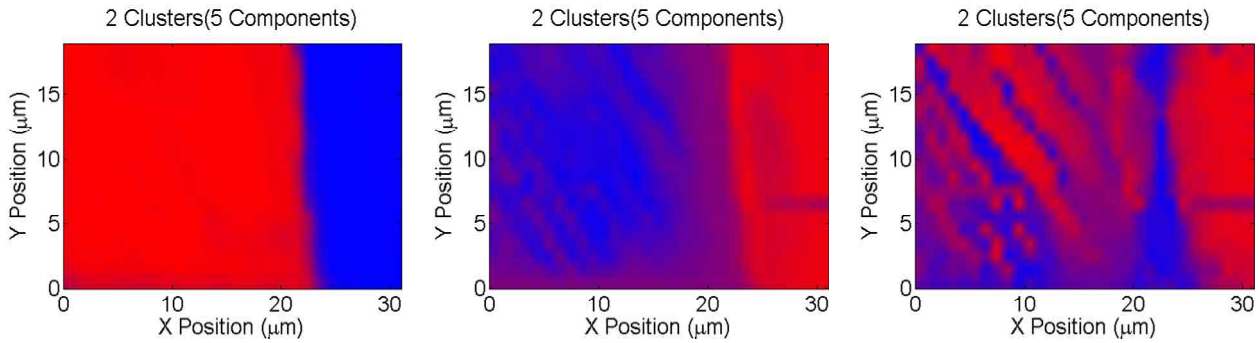
The computing platform is a PC with Win XP, Pentium 4 - 2.8GHz, and 1GB RAM. We used MATLAB - v7.2 as the software tool for the implementation of our clustering system.

3.2 Clustering results after ICA or PCA

Firstly, we did the experiment of direct clustering using all the raw dataset. Next, we also did it in case of clustering the scores based on the extracted components from the dataset by PCA or ICA. In our experiment, we used NIPALS-PCA and JADE-ICA for the extraction of main components. We also measured the clustering time for the each method for comparison.

The Fig. 3(a),(b),(c) to 6(a),(b),(c) show clustering results of each method, in cases of using all the dataset directly and using the score information based on the extracted components by PCA or ICA, respectively. For the clustering of the scores of extracted components, we firstly extracted 5 components from all the raw dataset and we did clustering based on their score information.

In case of Fig. 3(a), it is displayed after clustering about one thousand raw dataset into two clusters. The detail information of the dentin area located at left 2/3 region in the Figure is not shown. However, Fig. 3(b), (c) show the result of PCA and ICA after clustering into two clusters 5 main components extracted from the raw dataset. They present the dentinal tubules with about 135 degree angle direction. In Fig. 3(c), the case of ICA shows better detail separation of dentinal tubules than PCA clustering of Fig. 3(b).



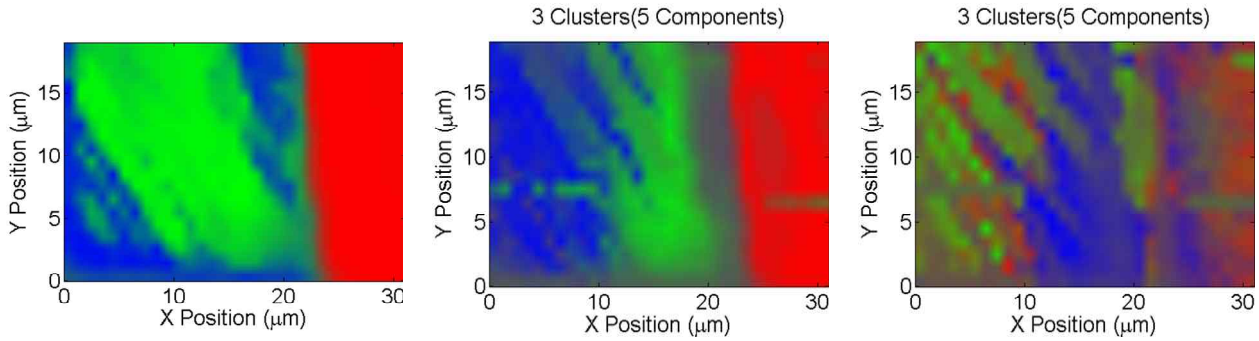
(a) clustering directly with all data (b) clustering after PCA (c) clustering after ICA

Fig. 3. Example of clustering of 2 clusters based on each method.

In case of Fig. 4(a) using all dataset, the dentin area is not still properly displayed because the huge raw dataset interact with each other negatively. In Fig. 4(b), (c) of PCA and ICA, they show better dentinal separation than that of Fig. 4(a).

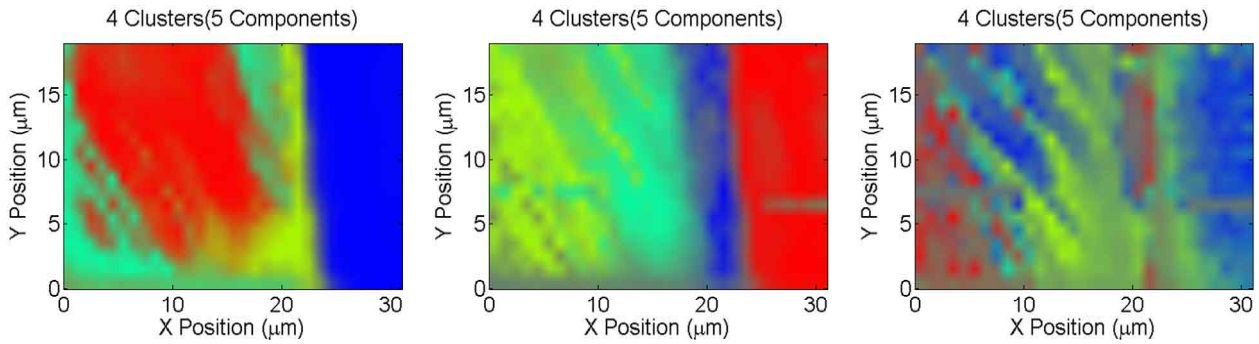
In Fig. 5, the result is almost same trend that of Fig. 4 except the number of clusters. Fig. 5(c) of ICA present more detailed dentinal tubule structure than Fig. 5(b) of PCA.

In Fig. 6, the clustering results show similar results with Fig. 5. Through the Fig. 3 to Fig. 6, we could find more detailed internal characteristic of dentin in case of clustering with ICA or PCA, compared with the case of using all the dataset directly. It also seems that cases of ICA show better dentinal tubule separation than those of PCA because



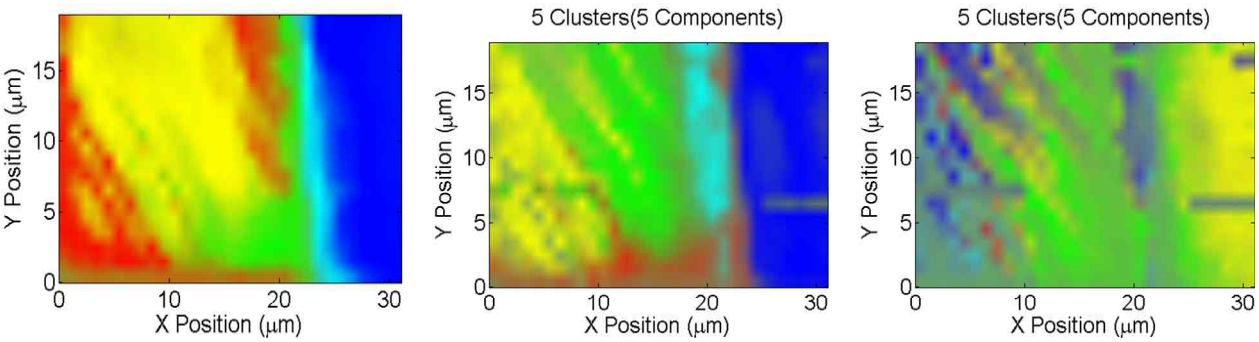
(a) clustering directly with all data (b) clustering after PCA (c) clustering after ICA

Fig. 4. Example of clustering of 3 clusters based on each method.



(a) clustering directly with all data (b) clustering after PCA (c) clustering after ICA

Fig. 5. Example of clustering of 4 clusters based on each method.



(a) clustering directly with all data (b) clustering after PCA (c) clustering after ICA

Fig. 6. Example of clustering of 5 clusters based on each method.

of the characteristic of ICA.

The following tables represent the processing time for clustering by each method. Through the experiment above, we found that ICA is useful along with PCA in terms of analysis, but if it takes much processing time, it is not applicable in the practical dental analysis software tools. When dental experts use the analysis software tool, if the response time is within about 2 to 3 sec, they would not be inconvenient.

Table 1 shows the clustering time, according to the number of clusters and each run, in case of using all the dataset directly.

Table 2, 3 show the processing time of clustering, according to the number of clusters and each run, in cases of using their scores after PCA and ICA, respectively.

In Table 4, it shows total processing time of each method. The method of all data does not need pre-processing time because it does not require the pre-processing step. However, PCA and ICA have preprocessing time before clustering. We first extract 5 main components from all dataset respectively and then apply them to the clustering step. ICA takes more pre-processing time, compared with PCA.

Through Table 1 to 4, we can find the following results: the case of using all the dataset directly

Table 1. Processing time of clustering using all data directly [sec]

Data	# of Class	Run1	Run2	Run3	Run4	Run5	Avg. Time
All data	2	1.77	1.65	1.66	1.65	1.77	1.70
	3	8.44	7.68	6.92	8.09	8.50	7.92
	4	10.98	11.26	11.29	11.69	10.28	11.10
	5	29.73	35.65	37.53	35.52	33.44	34.37

Table 2. Processing time of clustering after PCA [sec]

Data	# of Class	Run1	Run2	Run3	Run4	Run5	Avg. Time
PCA	2	0.7464	0.7654	0.7282	0.7494	0.7488	0.75
	3	0.8676	0.9271	0.9549	1.1026	0.9507	1.00
	4	1.0637	1.078	1.1573	1.092	1.0009	1.08
	5	1.3051	1.4194	1.4341	1.2589	1.4614	1.38

Table 3. Processing time of clustering after ICA [sec]

Data	# of Class	Run1	Run2	Run3	Run4	Run5	Avg. Time
ICA	2	0.63	0.6347	0.6232	0.6268	0.6529	0.63
	3	0.63	0.65	0.63	0.64	0.64	0.64
	4	0.72	0.68	0.66	0.68	0.69	0.69
	5	0.71	0.68	0.74	0.68	0.70	0.70

Table 4. Total processing time of each method [sec]

Data	All data				PCA				ICA			
# of class	2	3	4	5	2	3	4	5	2	3	4	5
Pre-processing time	0				0.28				1.41			
Processing time	1.70	7.92	11.10	34.37	0.75	1.00	1.08	1.38	0.63	0.64	0.69	0.70
Total time	1.70	7.92	11.10	34.37	1.03	1.28	1.36	1.66	2.04	2.05	2.10	2.11

requires much processing time for clustering, compared with the cases of using the scores after extraction of components by PCA or ICA. For example, the case of all the dataset requires about 16 to 21 times more than the case of PCA and ICA in 5 clusters. The reduction of total processing time of PCA and ICA comes from the usage of extracted score value from all raw dataset.

On the other hand, the clustering time of using the scores after PCA and ICA presents not much difference. However, as the number of cluster increases, the case of ICA relatively shows slow increase the processing time of clustering, compared with the case of PCA.

4. CONCLUSION

In this research, we studied on the clustering of hyperspectral Raman dentin data based on PCA and ICA approach for dental data analysis. The practical Raman hyperspectral data was captured by HR800 micro Raman spectrometer at UMKC-CRISP. The experimental hyperspecral data consists of 569 local observation points and each point has 1,005 spectral data.

We firstly clustered all the hyperspectal dataset directly. Next, we extracted the 5 components from the hypersectral dental dataset by PCA or ICA, and then did clustering over the dataset using their scores. We also measured the clustering time of each approach.

Through experiment, the cases of using the scores after the extraction of components by PCA and ICA showed more detailed information on the dentin internal structure than the case of using all the data directly. Furthermore, the cases of using the scores by PCA and ICA saved much clustering time up to 21 fold times, depending on the number of clusters, compared with the case of using all the dataset directly.

In comparison between the PCA and ICA based approaches, the case of ICA showed relatively the detailed information of dentin internal characteristic. It also showed that the case of ICA kept almost similar clustering time, while the case of PCA relatively shows the increase of the clustering time, as the number of cluster increases.

Therefore, for the huge hyperspectal data analysis, ICA based approach will be one of the effective approaches, in addition to PCA based approach. It can not only give more detailed information in terms of medical aspect but also save the much clustering time for the medial data analysis.

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