

A Study on Data Classification of Raman OIM Hyperspectral Bone Data

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ABSTRACT

This was a preliminary research for the goal of understanding between internal structure of Osteogenesis Imperfecta Murine (OIM) bone and its fragility. 54 hyperspectral bone data sets were captured by using JASCO 2000 Raman spectrometer at UMKC-CRISP (University of Missouri-Kansas City Center for Research on Interfacial Structure and Properties). Each data set consists of 1,091 data points from 9 OIM bones. The original captured hyperspectral data sets were noisy and base-lined ones. We removed the noise and corrected the base-lined data for the final efficient classification. High dimensional Raman hyperspectral data on OIM bones was reduced by Principal Components Analysis (PCA) and Linear Discriminant Analysis (LDA) and efficiently classified for the first time. We confirmed OIM bones could be classified such as strong, middle and weak one by using the coefficients of their PCA or LDA. Through experiment, we investigated the efficiency of classification on the reduced OIM bone data by the Bayesian classifier and K-Nearest Neighbor (K-NN) classifier. As the experimental result, the case of LDA reduction showed higher classification performance than that of PCA reduction in the two classifiers. K-NN classifier represented better classification rate, compared with Bayesian classifier. The classification performance of K-NN was about 92.6% in case of LDA.

Key words: Data lassification, Data reduction, Hyperspectral Data, Raman Spectrometer

1. INTRODUCTION

Along with modern advanced medical techniques and equipments, the diseases which were hard to treat years ago are relatively easy. Osteogenesis Imperfecta (OI) is a genetically and clinically heterogeneous disease giving to the tissue abnormality and bone fragility. It relates with the abnormal presence of Type I collagen. This type collagen comes from genetic mutations [1]. However, the specific mechanism is under ill-defined. The researches on this problem still continue and some results come out. One of the recent

known results is the bone fragility due to abnormal mineral-matrix interactions [2].

However, in order to solve this problem, further academic and clinic research to understand the mechanism along with related instruments is needed. Raman spectrometer is one of the instruments to effectively diagnose bone and its related disease. It can provide hyperspectral data on bone specimens.

The hyperspectral data is an extensive data gathered in the wide electromagnetic spectrum domain [3]. As a simple example for easy understanding, a human can see only visual light band. However, a mantis shrimp can see not only it, but also the broad bands from ultraviolet ray band to infrared ray band. Therefore, this mantis shrimp with a wider band than a human, can distinguish a prey or an object better in the water. The hyperspectral data can be different from a multispectral data which has tens to hundreds bands, because

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the hyperspectral data contains from hundreds to thousands bands.

Some typical research areas of hyperspectral data are remote sensing, agriculture, military and electronic micro scope related medical area etc. These have been a center of attraction since the mid of 1980s [4]. Figure 1 shows an example of hyperspectral data profile captured from an OIM bone specimen by JASCO 2000 Raman spectrometer at UMKC-CRISP.

Hyperspectral data has n -dimensional spectrum data regarding a spot, which represents the characteristic of the spot in the spectrum [5]. In Figure 1, an interpretation of a bone's internal structure can be partly possible in terms of biochemical realm by analyzing the distributed shapes in the spectral profiles of OIM bone specimens.

We briefly introduced the hyperspectral data handling technique into bone classification [6]. In this work, for the practical research to understand the internal structure of OIM bone and its fragility, we describe how to get useful hyperspectral data practically from OIM bone specimens by JASCO 2000 Raman spectrometer at UMKC-CRISP. We introduce the detailed data acquisition and preprocessing such as smoothing and base-lining for the captured hyperspectral data. And then we reduce the high dimensional hyperspectral data by PCA and LDA techniques. We show the distribution of PCA and LDA coefficients in 3 di-

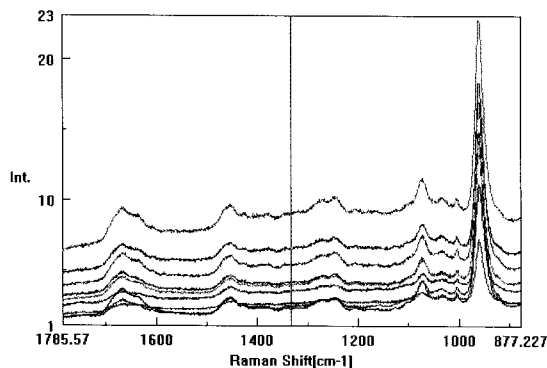


Fig. 1. Example of hyperspectral data from OIM bones.

mensions to demonstrate the possibility of OIM bone classification. Finally we classify it by using Bayesian classifier and K-NN classifiers for biochemical interpretation for the internal structure of OIM bone.

This paper is organized as follows: In Section 2, we explain our system for classifying OIM hyperspectral data. In Section 3 and 4, we mention the data reduction of hyperspectral data and classifiers, respectively. In Section 5, we discuss the experimental results and finally we conclude our research in Section 6.

2. OUR SYSTEM FOR CLASSIFYING OIM HYPERSPECTRAL DATA

The system block diagram is presented in Figure 2. At first, hyperspectral data on OIM bone specimens is acquired by a spectroscopy such as a JASCO 2000 Raman spectrometer, and stored in a medical hyperspectral database.

Secondly, some preprocessing steps such as smoothing and base-line correction, etc. are needed to remove noises and fluorescence effect which can occur in the data acquisition process. On the other hand, hyperspectral data has so huge dimension that it is not easy to directly analyze the data. In our research, the dimension of OIM hyperspectral data is about 1,090. Therefore, thirdly, we need a step to reduce the dimensionality of data and to extract important information from such an ex-

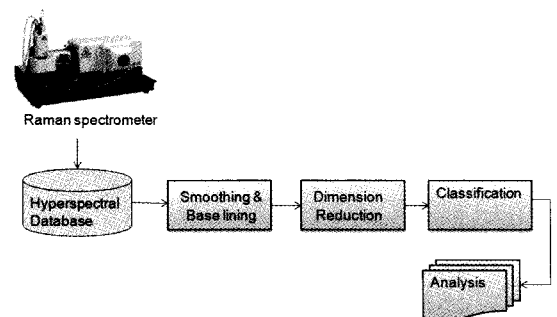


Fig. 2. The system block diagram for classification of OIM data.

tensive hyperspectral data. In general, statistic methods like PCA or LDA can be used.

Fourthly, we apply the classification step to the reduced data which may represent the features of OIM bones. Finally, in the analysis step, we can put biochemical interpretation and clinical meaning on the OIM bone groups, based on the classified data.

In this research, we classify a hyperspectral data for the final biochemical interpretation through the analysis step.

2.1 Hyperspectral data acquisition

Firstly, hyperspectral data is acquired from OIM bones by JASCO 2000 Raman spectrometer and stored in the medical database. In order to make the necessary information processing easy afterward, we need to do the file conversion from JWS file format to the general text format, because the stored data JWS file is JASCO's specific file format. JASCO company only support the file extension of *.jws.

After converting the JWS formatted hyperspectral data into text formatted data, we need to observe the text file structure. Figure 3 presents an example of a part of converted text format from

```

1  TITLE      ym019-wt-oim
2  DATA TYPE
3  ORIGIN     JASCO
4  OWNER
5  DATE       108/05/29
6  TIME       17:24:37
7  SPECTROMETER/DATA SYSTEM
8  RESOLUTION
9  DELTAX     0.833341
10 XUNITS     1/CM
11 YUNITS     Int.
12 FIRSTX    877.2269
13 LASTX     1785.5684
14 NPOINTS   1091
15 FIRSTY    0.29033
16 MAXY      11.89382
17 MINY      0.01641
18 XYDATA
19 877.2269   0.290326
20 878.0602   0.240185
21 878.8935   0.250602
22 879.7269   0.249823
23 880.5602   0.272028
24 881.3936   0.273457
25 882.2269   0.201831
26 883.0603   0.212268
27 883.8936   0.23624

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Fig. 3. Example of a part of text file format for Raman hyperspectral data

the captured hyperspectral data by JASCO 2000 Raman spectrometer. We can get it by a software tool, Spectra Analysis purchased with JASCO 2000 Raman spectrometer.

As the result of the text file observation, we found that the front 18 line part of the data showed the file head information. After the head information, there were about 1,090 pairs of Raman shift frequency and corresponding data in sequence. With this information of the text file structure, we can extract the hyperspectral data easily.

2.2 Noise removing and base-line correction

The first acquired hyperspectral data from OIM bones by Raman spectrometer is partly contaminated by noises and fluorescence effect [7], as you can see in the left down corner of Figure 4. Therefore, for the sake of effective classification of OIM bone data, these things should be removed before the classification steps. In this research, we use a mean filter and a base-line correction by Spectra Analysis tool shown in Figure 4 for noise removing and fluorescence effect removing, respectively.

The simple base-line correction by Spectra Analysis, which based on the two extreme end-points, is not enough to completely remove fluorescence effect. Additionally, even if multipoint base-line correction is available in Spectra Analysis, it is not easy to apply it to our research, because keeping consistency of the each local point

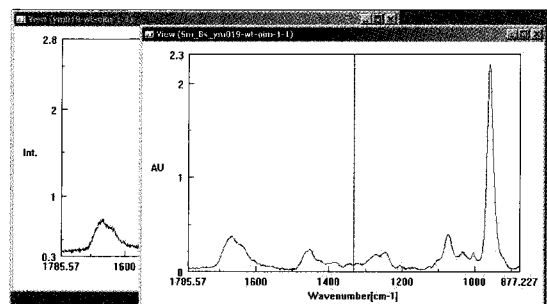


Fig. 4. Example of noise removing and base-line correction.

location is not easy. And further more, this requires lots of manual processing. Therefore, to cope with this problem, finally we decided to use the first derivative of the noise-removed and based-line corrected hyperspectral data for the afterward data processing.

3. DIMENSIONAL REDUCTION OF HYPERSPECTRAL DATA

Hyperspectral data contains huge dimensional data. OIM hyperspectral data used in our research also has 1,091 dimensions. If we directly process this high dimensional data, it takes long processing time and it is hard to expect an efficient data processing because of Hughes phenomenon [8]. Therefore, we need a dimensional reduction step which does not only reduce the data dimension but also extract salient features from the original huge data set. For these purposes, statistical methods such as PCA, LDA can be used.

3.1 Data reduction by PCA

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 the discrete Karhunen-Loève Transform (KLT) or the 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 data set 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 [9].

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 was suggested by Herman Wold in 1966. We selected it in our research, because it could extract as many principal components as we wanted to extract from hyperspectral data set. The following is its algorithm description.

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

1. initial assumption for the principal component,

$$t_{temp}$$

2. calculate the corresponding score,

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

3. calculate the normalized score, $p = \frac{p_{temp}^T}{\|p_{temp}^T\|}$

4. recalculate the principal component, t using the

$$\text{score, } t = \frac{X p}{p^T p}$$

5. if $|t - t_{temp}| < \text{tolerance}$, go to step 6,

Otherwise, $t_{temp} = t$ and go to step 2

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 for calculation of the next component

3.2 Data reduction by LDA

LDA is almost same to Fisher's Linear Discriminant (FDA) by Fisher in 1936. So, people often used them interchangeably. In general, PCA and LDA have been commonly used for data classification and dimension reduction. For maximal separability to the given data set, LDA maximizes the ratio of between-class variance and the within-class variance. The main difference between

LDA and PCA is that LDA does for data classification and PCA does for feature classification. In other words, in LDA, the shape and location of the original data set are not changed. It tries to provide more class separability by drawing decision boundaries, but PCA changes them when transformed to a different space [9]. The following is the procedure of LDA algorithm [10].

C = the number of classes

μ_i = the mean vector of class i , $i = 1, 2, \dots, C$

M_i = the number of sample within class i , $i = 1, 2, \dots, C$

$M = \sum_{i=1}^C M_i$, the total number of samples

$\mu = 1/C \sum_{i=1}^C \mu_i$, the total mean of samples

1. calculate Within-class scatter matrix,

$$S_w = \sum_{i=1}^C \sum_{j=0}^{M_i} (y_i - \mu_i)(y_i - \mu_i)^T$$

2. calculate Between-class scatter matrix,

$$S_b = \sum_{i=1}^C (\mu_i - \mu)(\mu_i - \mu)^T$$

3. for the computation of *Maximizing* $\frac{\det(S_b)}{\det(S_w)}$,

solving the generalized eigenvector problem

$$\text{such as: } S_b V = \lambda S_w V, \quad \lambda V = S_w^{-1} S_b V,$$

4. if S_w^{-1} exists, obtain a conventional eigenvalue problem: run $[V, \lambda] = \text{eig}(S_b, S_w)$, and go to 6. But, if not, singular problem occurs.

5. to avoid singular problem, first do PCA and reduce the dimensionality to a certain degree. And run $[V, \lambda] = \text{eig}(S_b, S_w)$.

6. select m -coefficients from n -coefficients of λ having the same dimension as input n -dimension, and by using m - V vectors corresponding the selected m - λ coefficients, reduce the dimensionality by product the selected m - V and input n -dimensional data.

4. CLASSIFIER FOR THE REDUCED HYPERSPECTRAL DATA

4.1 Bayesian classifier

Bayesian classifier is based on Bayesian theorem by Thomas Bayes in 1700s, which uses prior probability and conditional probability of likelihood probability to get posterior probability.

The following example is an easy illustration regarding the principle of Bayesian classifier [11]. Suppose that total 60 green and red beans are classified according to their weight and length. When some unknown beans come in, one decides the category that each unknown beans should belong to, using the existing heuristic information. If the number of green beans is two times more than red beans, some beans which newly come in have two times higher probability, which may belong to green category. In Bayesian classification, we call this probability as prior probability. Prior probability is based on the experience so far. Therefore, we can estimate the category to which unknown input beans would belong. That is,

Probability of green bean = *number of green bean* / *number of total bean* = 40/60,

Probability of red bean = *number of red bean* / *number of total bean* = 20/60.

If we firstly get prior probability, we need to check the label of neighbor beans for the likelihood of a newly input bean. Therefore, after we check the label of neighbor beans of a new given bean, we can calculate the likelihood of the given bean as follows:

Green likelihood of a given bean = *number of green bean among neighbor beans*

/ *total number of green bean,*

Red likelihood of a given bean = *number of green bean among neighbor beans*

/ *total number of green bean.*

Suppose that there are one green bean and three red beans around a given bean, then the newly input bean, x has a probability of being green, $1/40$, a probability of being red, $3/20$. Therefore, in prior probability, x has higher probability of being green, but in likelihood probability, it is opposite. In Bayesian classification, the final decision has done based on above two kinds of information; that is, to decide final posterior probability, we use prior probability information and likelihood probability information.

Posterior probability of green to a given bean
 = prior probability of green * green likelihood
 probability of a given bean = $4/6 * 1/40 = 1/60$

Posterior probability of red to a given bean
 = prior probability of green * red likelihood
 probability of a given bean = $2/6 * 3/20 = 1/20$

If we express this principle into a generalized form based on the above example, let variable $X = \{x_1, x_2, \dots, x_d\}$, and category $a_i = \{a_1, a_2, \dots, a_d\}$. Then category a_i has a posterior probability as follows:

$$p(\omega_i/X) = p(\omega_i) \prod_{k=1}^d p(x_k/\omega_i) \tag{1}$$

Because we decide the category based on this probability, we can define a decision function $g_i(X)$ as followings:

$$g_i(X) = \ln p(\omega_i) + \ln \prod_{k=1}^d p(x_k/\omega_i) \tag{2}$$

If $p(x)$ is assumed a Gaussian distribution,

$$\ln \prod_{k=1}^d p(x_k/\omega_i) = -d/2 \ln \pi - \ln \left| \sum_i |1/2 - (x - \mu_i)' \sum_i |^{-1} (x - \mu_i)/2, \tag{3}$$

$$g_i(X) \cong \ln p(\omega_i) - \ln \left| \sum_i |1/2 - (x - \mu_i)' \sum_i |^{-1} (x - \mu_i)/2$$

Therefore, category classification for the newly input data is possible by using the decision function $g_i(X)$.

4.2 K- NN classifier

K-NN classifier is a simple one of machine learning algorithms. The basic principle is that a newly input can be classified by the majority voting of K-nearest neighbors. In general, K is integer and not large number.

The selected neighbors have been correctly classified. Even though there is no separated training procedure, implicitly one thinks this existing classified information as a sort of training. In order to recognize the neighbors of the input data, the data is displayed and one computes the distance between the input and K-nearest neighbors in the multidimensional feature space. Many different distance measures can be used, but generally one may use a simple measure of Euclidian distance or Manhattan distance [12].

Basically, K-NN classifier is sensitive to the local data structure, because it decides the category by considering K-nearest neighbors to the input data. The following equation shows the computation for the majority voting.

$$p(\omega_i/X) = \frac{p(X, a_i)}{\sum_{j=1}^c p(X, \omega_j)} \cong \frac{K_i}{K} \tag{4}$$

Where, K is the selected K neighbors, K_i is the number of data which belong to ω_i category. Input data X will be classified into ω_i category which has the largest number of K_i .

The following equations present the *Euclidian distance* and *Manhattan distance*, respectively. *Manhattan distance* is also called as *city block distance* which is based on a form of taxicab geometry.

$$\text{Distance } D(a, b) = \sqrt{\sum_{i=1}^n (a_i - b_i)^2} ; \text{Euclidian distance} \tag{5}$$

$$\text{Distance } D(a, b) = \sum_{i=1}^n |a_i - b_i| ; \text{Manhattan distance} \tag{6}$$

Where, D is the distance between two points, a and b which locate in n -dimensional feature space.

5. EXPERIMENTAL RESULTS AND DISCUSSION

5.1 Experimental environment

In our research, OIM bone specimens came from University of Missouri-Columbia. They consist of three genotypes: normal wild bone, *wt* and middle strength bone, *oim/+* and weak bone, *oim/oim*. We acquired hyperspectral data from the bone specimens by JASCO company's 2000 Raman Spectrometer at UMKC-CRISP.

The acquired data are 54 hyperspectral data sets that each data set has 1,091 data points. The Figure 5 shows an example of OIM bone specimens.

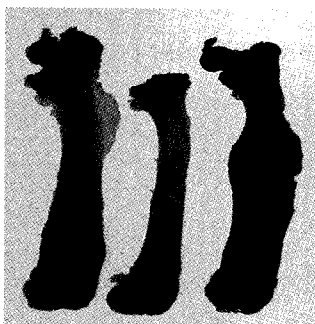


Fig. 5. Example of OIM bone specimen.

We used a PC with Win XP, Pentium 4 - 2.8GHz, 1GB RAM, as a computing platform and JASCO Spectra Analysis and MATLAB - v7.2 as software tools.

5.2 Noise removing and base-line correction

Firstly, in order to remove noises for all the acquired OIM hyperspectral data, we used a mean filter with window-size 9 built in JASCO Spectra Analysis tool. Figure 6 presents an example of the acquired hyperspectral data. Figure 7 shows the hyperspectral data after the noise removal.

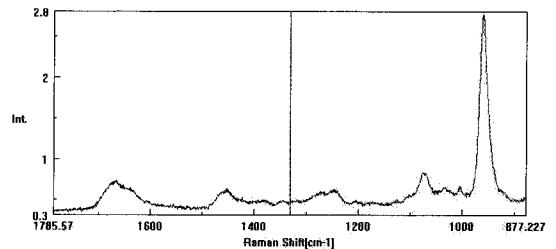


Fig. 6. Example of acquired noisy hyperspectral data.

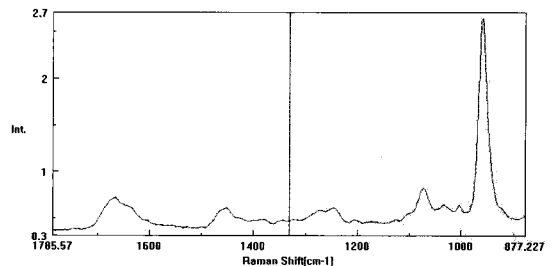


Fig. 7. Example of hyperspectral data after noise removal.

Next, we did base-line correction to eliminate fluorescence effect which could occur in the data acquisition process, like an example of Figure 8, because fluorescence effect usually still remains within the acquired hyperspectral data after noise removal.

To completely remove non-linear bias like fluorescence effect, we may use multipoint base-line

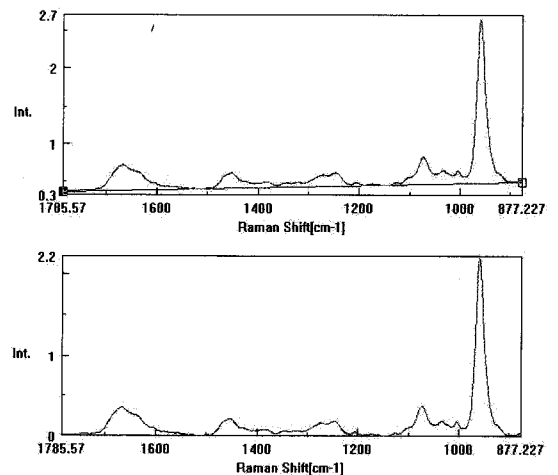


Fig. 8. Example of hyperspectral data with base-line correction.

correction by using Spectra Analysis tool. However, it is difficult to keep consistency to every hyperspectral data and to handle vast data by the manual operation.

Therefore, in this research, in order to eliminate non-linear bias, we took the first derivative on the data after noise removing. Then, we got the noise and bias removed data set, so called the pure hyperspectral data set for effective OIM data classification.

5.3 Dimensional reduction by PCA and LDA

For the hyperspectral data for effective classification, firstly we reduce 1,091 dimensions to 3 dimensions by PCA. In this research, we used 3 dimensions because the first 3 coefficients of PCA had about 98.25% power of all the energy of given hyperspectral data.

In case of LDA, we could suffer singular problem in the process of handling 1,091 huge dimensional matrixes directly. So we adopted PCA to firstly reduce the high dimensionality to a certain degree, and then applied LDA to it. In this research, we reduced high dimensional data into 10 dimensions data by PCA, and finally we got 3 dimensions of hyperspectral data by LDA.

Figure 9 and 10 show the reduced 3 dimensional coefficient distributions of PCA and LDA,

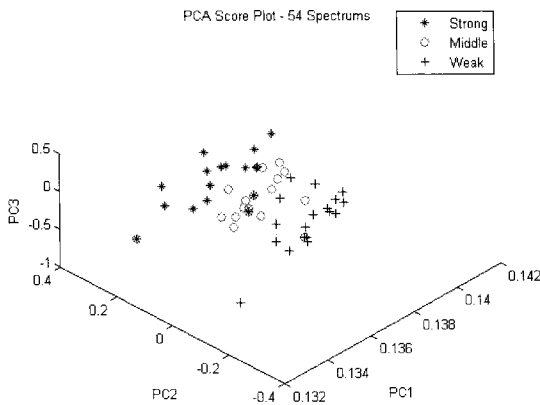


Fig. 9. PCA coefficient distributions in three dimensions.

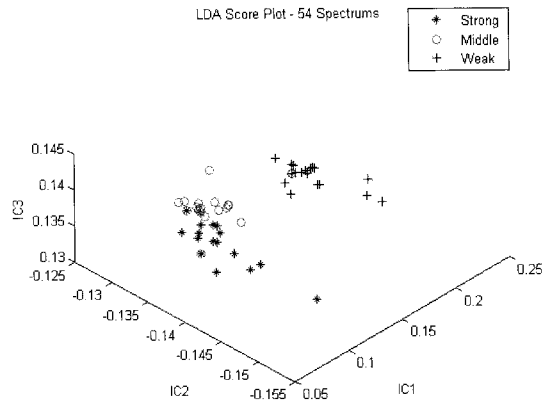


Fig. 10. LDA coefficient distributions in three dimensions.

respectively. In Figures, we could see the classification possibility of OIM bones.

5.4 Classification performance comparison of classifiers

Table 1 shows the performance of classifiers according to data reduction methods. We adopted a cross-validation technique because we had 1,092 huge high dimensional data, but we only had 54 hyperspectral data sets. In order to measure the classification performance of each approach, we used 3-fold method as the cross-validation method.

In case of LDA reduction, we found high classification performance of about 92.6 % in K-NN classifier. Each classifier showed higher performance than that of PCA. Bayesian classifier yields about 13% and K-NN about 3.7% better performances than each case of PCA reduction. So, we presumed that LDA showed better performance because it had built-in characteristic for efficient between-category classification.

Table 1. Comparison of classification performance (%)

Data Reduction Method		PCA	LDA
Classifier	Bayes	75.9	88.9
	K-NN	88.9	92.6

In case of PCA reduction, K-NN classifier presents 88.9% classification rate. It is about 13% higher performances than Bayesian classifier.

Therefore, high dimensional reduction of hyperspectral data through LDA and classification procedure shows better classification performance than that of PCA in our research. On the other hand, K-NN classifier presents better performance than Bayesian in both LDA reduction and PCA reduction.

6. CONCLUSION

In this research, in order to know OIM bone internal structural property, we got 54 data sets of 1,091 dimensional OIM hyperspectral data by JASCO 2000 Micro Raman Spectrometer at UMKC-CRISP. After some preprocessing such as noise removing and base-line correction, we got pure hyperspectral data. We reduced the pure hyperspectral data by PCA and LDA. So, we could confirm the classification possibility by the coefficients of PCA and LDA. Finally we classified Raman OIM hyperspectral data. We measured the performance of Bayesian and K-NN classifiers using the reduced data set.

As results of experiment, the data reduction approach using LDA shows about 92.6% high classification rate in K-NN classifier. That is, in case of data reduction by LDA, Bayesian classifier presents about 13% higher and K-NN classifier about 4% higher performance than those performances in case of PCA reduction.

In our research, K-NN classifier shows better performance than Bayesian classifier. We think that it means the data distribution of PCA and LDA coefficients in this experiment does not always follow Gaussian distribution.

In case of data reduction by LDA, because LDA has a good classification characteristic of between-classes, the classification performances of Bayesian classifier and K-NN classifier are higher

than those cases of PCA reduction.

As further research, we will pursue the internal bone structural analysis based on our classified hyperspectral data distribution. Namely, the deeper biochemical interpretation is needed for the internal bone structure. The finding out the main cause of OIM, in terms of the view points including bone internal matrix and its biochemical characteristics, is also needed.

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