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Blood Glucose Detection from Infrared Spectral Data by Gaussian Single-Peak Fitting

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Abstract

Infrared spectra contain abundant information on the structure of the material. It requires fewer samples for detecting the composition of matter. The characteristics of infrared spectroscopy technology enhance its wide use in biomedical, materials, food testing and criminal investigation science, etc. This paper presents a method for analyzing infrared spectra data based on Gaussian single-peak fitting. Firstly, recognition and peak shape extraction algorithm of Fourier transform infrared spectra for Gaussian fitting is proposed. Secondly, the method is applied to extract specific infrared spectra data from the control group and the experimental group in order to obtain the sample data with different content of blood glucose. Finally, the Gaussian single-peak fitting method was applied to analyze the infrared spectra data. By comparing its results with the second derivative spectra of infrared absorption spectra, the results show that the Gaussian single-peak fitting is not only effective for detecting the glucose in blood, but also very important for processing the Infrared spectroscopic data, which can provide further application of infrared spectroscopy detection technology.

1. Introduction

Various types of spectral analysis methods have been widely used in many fields, especially in the field of life science for it can describe the phenomenon of micro-life well [1]. In the field of infrared spectroscopy, it has been widely used in the field of medical diagnosis. And there are many types of diseases that can be diagnosed by infrared spectroscopy technology. For example, Joanna Depciuch used this technique to study the relationship between phospholipid and protein levels in serum of patients with major depression. FTIR spectrum and its second-order derivative spectra show that the phospholipids can affect the structure and function of the related proteins. So, the author attends to think the FTIR technique can be used as a tool for assessing depression [2]. In the diagnosis of cancer area, Hui Liu et al examined A1653 / A1543 (protein secondary structure), A1543 / A2958 (relative content of protein and lipid) and A1106 / A1166 (structure and content of sugar) in erythrocyte of gastric cancer via peak value ratio of infrared spectroscopy. The results of the study show that there are differences in protein secondary structure and sugar structure between gastric cancer patients and healthy people. That is, FTIR spectroscopy can be used to diagnose gastric cancer [3], and in recent years there are many other techniques related to infrared spectroscopy useful in cancer diagnosing and identification [4]. Mohammdreza introduced a method based on

attenuated total reflection-Fourier transform infrared spectroscopy combined with classification method in the diagnosis of renal failure disease. The focus of the study is on the 900-2000 cm^{-1} of the infrared spectrum with blood sample. Quadratic Discriminant Analysis (QDA) combined with the ATR-FTIR spectroscopy technology is proved to be a effective method in distinguish serum samples from patients with renal failure and healthy subjects [5]. To assess the toxicity of cyanide on reproductive systems, Shiddappa *et al.* used FTIR to study the toxic effects of cyanide on the molecular level of rat spermatozoa. In the course of the study, the second-order derivative spectra of infrared spectroscopy were used to analyze the biochemical composition and protein structure changes. The results suggest that FTIR spectral technology may provide an effective tool for cyanide reproductive system toxicity research [6]. At the same time, Fourier transform infrared spectroscopy in recent years is usually used to diagnose Parkinson's disease [7]. Many studies shown thatmore and more scholars pay attention to the application of infrared spectroscopy in medical detection and testing in recent years, and that infrared spectroscopy related technology has a wide application value in biomedical engineering.

In the field of blood glucose testing, Miguel Pleitez uses a mid-infrared quantum cascade laser to design a non-invasive blood glucose detector that can obtain spectral signals from the skin (two infrared wavelengths of 1054 cm^{-1} and 1084 cm^{-1}), this signal can be used to determine the body's glucose content [8]. In addition, FTIR spectral analysis combined with the principal component analysis method can also be used to detect different types of sugar [9]. Sherif S. Mahmoud *et al.* study the influence of blood glucose level on the infrared spectrum of erythrocyte membrane via considering the instability of blood glucose levels in patients with type II diabetes mellitus. The results suggest that the occurrence of erythrocyte membrane disorders in diabetic patients which denoted by the infrared spectrum of the spectrum associated with vibration of phospholipid molecules in the interface region [10]. Shen YC *et al.* used the infrared light transmission method to quantitatively determine the glucose concentration in the blood and examine its second derivative spectra of the infrared spectrum in the range of 950-1200cm^{-1}. The results showed that for the blood samples from the single patient, substraction of the second derivative values at 1082cm^{-1} and 1093 cm^{-1} can be used to directly determine the glucose concentration in the blood [11]. In the previous studies, many scholars conduct the Peak Fitting of infrared spectrum data to carry out the content detection. However, in actual operation, the number of peaks must be set up manually for its uncertainty. In this paper, we design a single-peak extraction algorithm for infrared spectroscopy, which can automatically identify its half-width, and can effectively extract the infrared spectrum of peak and peak-related data. Further, the Gaussian fitting method was used to detect the blood glucose level.

2. Experiment Design

Twenty male Wistar rats (200 ± 10 g) were randomly divided into two groups: control group and experimental group. The experimental group was hyperglycemia group. In order to study the infrared spectrum characteristics of the blood of hyperglycemia rats, the experimental group was modeled by hyperglycemia. The method was as follows: intraperitoneal injection of alloxan (10 mg/mL), with the dose 200 mg/kg. all group was conduct normal feeding for 10 days in the same environment. Then, the rats were anesthetized by intraperitoneal injection. Blood (3-5 mL) was extract via left heart apex acupuncture. Blood samples were biochemical tests and measured by infrared spectroscopy (Nexus 670 Fourier transform infrared spectrometer manufactured by Thermo Nicholas). Biochemical test results of blood sugar with hyperglycemia group greater than 11mmol/L are defined as the hyperglycemia. The attachment of ZnSe liquid pool (optical path 0.023 cm) was used to measured infrared spectrum data, and the data is shown in Figure 1.

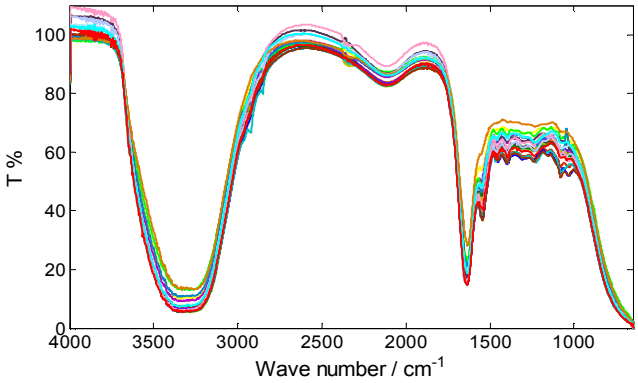

Figure 1. *Infrared spectra of blood samples.*

In order to ensure the accuracy of the measurement results, the infrared spectroscopy of background was collected at room temperature before the sample was measured. Then, the spectral data of blood samples were scanned with a resolution of 4 cm^{-1}, while subtracting the background noise by means of the difference spectrum method.

3. FTIR Spectral Peak Data Extraction and Its Gaussian Fitting

In order to identify the peak and its features better form spectral data, it is necessary to process the measured infrared spectrum data first. Here, the main processing is to perform baseline correction and automatic smoothing of all the infrared spectra. In order to display blood glucose levels of the samples, it is also necessary to convert the spectral data of each sample into its absorption spectrum. Here, 1500-1000 cm^{-1} of blood infrared spectrum was mainly considered for it contains lots of information, which is shown in Figure 2.

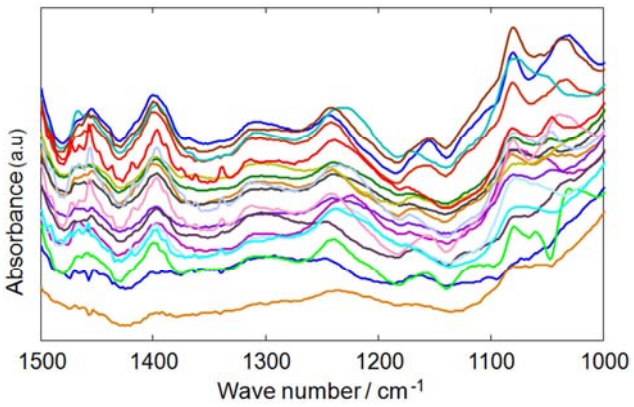

Figure 2. *Infrared absorption characteristics of blood in 1500-1000 cm^{-1} range.*

Figure 2 shows that blood samples have strong absorption peaks near 1082 cm^{-1}, 1230 cm^{-1} and 1400 cm^{-1}. The 1082 cm^{-1} absorption peak is often used to evaluate blood glucose levels [8, 10]. In order to be able to effectively analyze the peak, it is need to identify and extract the peak data first. According to the information of the peak and peak features of the infrared spectrum data, the determination algorithm of the peak position near the 1082 cm^{-1} is designed. The absorbance S (n) should satisfy the following conditions:

$$S(n)>S(n-1) \ \& \ S(n)>S(n+1) \quad (1)$$

At the same time, in order to meet the Gaussian fitting to the peak data, it is needed to set the infrared spectral data selection conditions, namely the formula:

$$S(n+i)>S(n+i+1) \ \& \ S(n-i)>S(n-i-1) \quad (2)$$

In the formula (2), i = 1, 2, 3,... k, where k is the data number of half-width, the value of k is 5 in this paper for the actual extraction of peak data. Together with the peak data, there are at least 11 fitting data points to meet the Gaussian fitting requirements, which can guarantee the validity of Gaussian fitting. For the infrared spectral peak data identification and extraction, it can also select the specific k value that is automatically identified half-width. Single-peak Gaussian fitting of Infrared spectral peak data can be completed by the formula (3):

$$f(x)=a\exp\left(-\frac{(x-b)^2}{c^2}\right) \quad (3)$$

Equation (3) is a single-peak function, and its parameters *a*, *b*, and *c* have important significance in fitting on the infrared spectral peak data. Here, *a* represents the amplitude of the fitting curve, the higher the value, the higher the peak, the more content of the corresponding material. The value of *b* represents the position of the position where the peak is fitted. The greater the value of *c*, the wider the peak shape, the more the corresponding substance content. Therefore, the results of the single-peak Gaussian fitting of the infrared spectrum data can also reflect the internal structure and composition of the sample.

4. Results and Discussion

In the detection of blood glucose via infrared spectroscopy technology, the contribution of other components in blood may largely affect the experimental results. These factors may cause changes in the spectral peak position, and cause the interference absorption peak shape, which could led to more difficult to extract blood glucose information. The composition of the blood is more complex, more ingredients will affect the absorption characteristics. In order to study the characteristics of IR spectra, the peak shape data of the experimental group and the control group were extracted for each with 20 samples, and then the mean value was obtained. Gaussian fitting of the extracted peak data is carried out on the Matlab platform. The fitting result is able to reflect the peak width and peak information of the peak shape (Figure 3). Figure. 3 shows the single-peak Gaussian fitting results of the peak data at 1082 cm^{-1} in the experimental and control groups, where the peak data information can better reflect the blood glucose content in the sample.

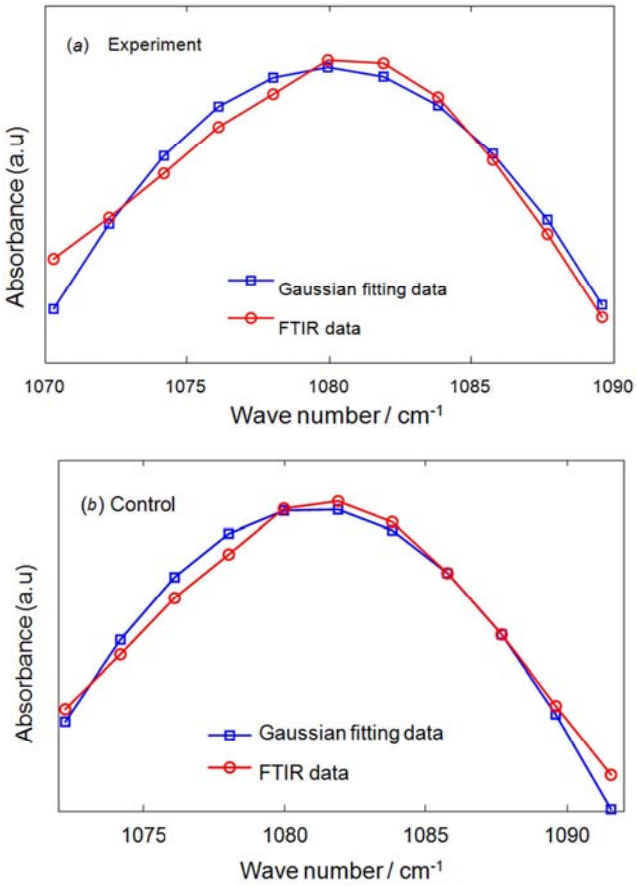

Figure 3. *Gaussian fitting of single FTIR peak (a) hyperglycemia group (b) control group.*

The results of the fitting data *a*, *b*, *c*, and *R-square* of each group are shown in Table 1, in which the value of parameters *a*, *b*, c and *R-square* of the control group and the experimental group are different. The experimental group has a large value of *a*, which indicates that the experimental group has a high peak at 1082 cm^{-1}. The fitting results show

that *b* has one wave number difference from each other. At the same time, from the fitting point of the value *c*, the experimental group of c value is about 2 times larger than the control group, namely the wave peak of infrared spectrum of experimental group at the 1082 cm^{-1} is wider, and the blood glucose content of the experimental group is more than the control group.

Table 1. *Gaussian Fitting Results of Infrared Spectral Peak Data.*

Parameters	*a*	*b*	*c*	*R-square*
Control	0.07411	1081	25.02	0.9794
Experiment	0.2696	1080	51.09	0.9497

In order to further verify the effectiveness of the above method, the second-order derivative spectrum of the test data was calculated by using Nicolet's Omnic software. The difference between the second-order derivative spectra of the experimental group and the control group was examined by using the second-order derivative spectrum analysis of the infrared spectrum 1082 cm^{-1} at the absorption peak (Figure 4). Using the second derivative of the infrared spectrum and combining the results of Gaussian fitting in Figure 3 and Table. 1, some insignificant constituent components and their structural information can be shown. Figure 4 shows the differences of second derivative of infrared spectra in blood sample of the hyperglycemia group and the control group.

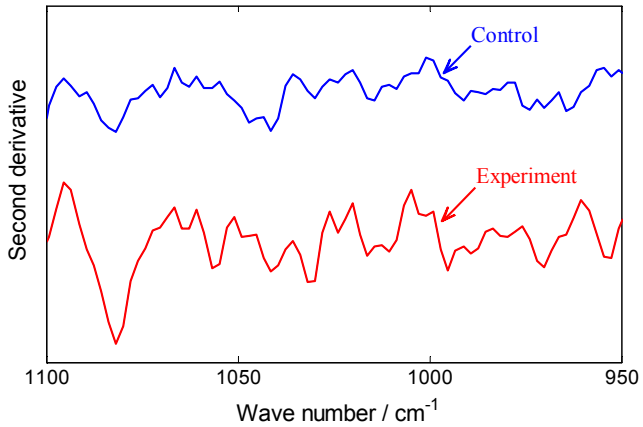

Figure 4. *Second derivative spectra of hyperglycemia and control group.*

Since there is no efficient method to analyze the typical overlapping peak information within the infrared spectral data, it is difficult to determine the characteristics of the infrared absorption peak. However, it can be seen from Figure 4 that the difference of the second-order derivative spectrum of the infrared spectrum of the experimental group and the control group, which reveal that the experimental group has a strong absorption peak near the 1082 cm^{-1}. At the same time, in the vicinity of 1065 cm^{-1}, the experimental group also showed strong absorption characteristics, the absorption at 1065 cm^{-1} is mainly caused by blood glucose from the perspective of ref [12].

Most of the blood glucose detection by infrared spectroscopy was conducted by measuring the absorption spectrum of blood tissue and the data analysis, and the spectral information reflecting the structure and state of glucose. Especially in the mid-infrared spectrum, and the infrared spectrum data can reflect the fundamental frequency of the vibrations of glucose molecules. The peak height ratio of different wave numbers is often used to analyze the infrared spectral data for the peak height ratio has certain feasibility. Because of the superposition characteristic of the infrared spectral, the Gaussian fitting method can explore the content of specific substances in the sample by peak quantitative research method, and can be more accurate than the peak height ratio quantitative analysis method.

5. Conclusions

Infrared spectroscopy is very effective in the field of material composition detection with strong pertinence, especially for the identification of molecular components of the sample. In the specific application of infrared spectroscopy technology, not only the composition of the sample can be qualitative analyzed, but also the quantitative characteristics of sample can be analyzed too. In this paper, we proposed a method for recognizing the peak of the infrared spectrum and the peak shape extraction algorithm. Then, the single-peak Gaussian fitting algorithm of the infrared spectral peak data was designed. The data were verified by the infrared spectra of the hyperglycemia group and the control group via the single-peak Gaussian fitting algorithm. The validity of the algorithm is discussed by analyzing the second derivative of the glucose absorption spectrum of 1065 cm^{-1} and 1082 cm^{-1} from each group. The result show that the single-peak Gaussian fitting method is consistent with the traditional method in the analysis of blood glucose content, and the method of single-peak Gaussian fitting method can be further extended in infrared spectroscopy application.

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