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Study on the Signal Processing and Analysis System of Micro-Spectrometer

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In order to study functions of spectral signal and intelligent spectrometer in materials analysis, this paper designs the signal processing and analysis test of micro-spectrometer. The study object is spectral signal. This paper deeply discusses about problems on signal processing and analysis techniques of micro-spectrometer, establishes a model structure of signal processing and analysis system of micro-spectrometer, deeply studies the selection of wavelength and spectral recognition problems, and puts forward corresponding algorithm and strategies. This paper also discusses the wavelength selection during quantitative analysis of spectral signal and puts forward the method for selecting segmented wavelength based on particle swarm optimization algorithm. Test results prove that this algorithm can be used to solve the subjective randomness for wavelength selection during quantitative analysis and complexity and slow convergence of the existing methods. In addition, this paper also researches the module transformation of spectral signal and puts forward that segmented direct correction method of support vector machine is used to solve data conversion problems of different spectrometers among measuring signals in different solutions under same measuring conditions, so as to provide basis for universality and comparability of measurement data of different spectrometers. It can be known herein that spectrum research experiment of micro-spectrometer lays a foundation for its application and development in each field in the future.

1. Introduction

Spectrometer is the important analysis instrument used to analyse the composition and content of substance by obtaining the spectral signal of the substance, which is widely used in many filed such as the military and scientific research etc (Ghita et al. , 2015). With the continuous development of science and technology as well as people’s increasing demands in measurement, the micro-spectrometer featured with micromation, integration and intellectuation has been the important direction for the development of spectrometer (Gomez-Nubla et al., 2017). The development of computer and artificial intelligence is the new content of stoichiometry, and also provides opportunity for the intelligence of spectrometer (Guarini et al., 2016). Artificial intelligence is the technology developed on the basis of disciplines such as nerve physiology, philosophy of language and computer science etc., and the objective of which is to simulate and realize the human intelligence with manual methods (Hathazi et al., 2014). Partial thinking function of human brain can be replaced by artificial intelligence technology, which lays solid theory foundation for the transition from traditional instrument with simple measurement to the modern instrument with intellectual analysis (He et al., 2016).

Chemometrics is an interdiscipline using the mathematical and statistical methods to design or select the optimal measuring procedure and experiment method, and to obtain the chemistry and its information to the maximum by analysing data (Hlaing et al., 2017). In recent years, the chemometrics has absorbed the latest achievements in fields such as computer and artificial intelligence etc. widely, which has been applied to the analytical instrument, so that the automation and intelligence level of analytical instrument have been improved continuously, and the working pressure of analysts has been reduced greatly, the working efficiency has been improved greatly ((Hoppe et al., 2017).

To study functions of spectral signal and intelligent spectrometer in materials analysis, this paper designs the signal processing and analysis test of micro-spectrometer. This paper deeply discusses about problems on signal processing and analysis techniques of micro-spectrometer, establishes a model structure of signal

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processing and analysis system of micro-spectrometer, deeply studies the selection of wavelength and spectral recognition problems, and puts forward corresponding algorithm and strategies. This paper also discusses the wavelength selection during quantitative analysis of spectral signal and puts forward the method for selecting segmented wavelength based on particle swarm optimization algorithm. Test results prove that this algorithm can be used to solve the subjective randomness for wavelength selection during quantitative analysis and complexity and slow convergence of the existing methods. In addition, this paper also researches the module transformation of spectral signal and puts forward that segmented direct correction method of support vector machine is used to solve data conversion problems of different spectrometers among measuring signals in different solutions under same measuring conditions, so as to provide basis for universality and comparability of measurement data of different spectrometers. It can be known herein that spectrum research experiment of micro-spectrometer lays a foundation for its application and development in each field in the future.

2. Multi component analysis and wavelength selection

Multi component analysis and wavelength selection is the basic problem in spectral analysis. The multicomponent analysis method based on support vector machine, uniform design, cross validation and wavelet analysis as well as the segmented wavelength selection method based on particle swarm optimization are proposed in this paper on the basis of common method of multi component analysis and wavelength selection; and the computer simulation method is also used in relevant method verification.

Table 1: Table of samples' concentration

No.		1	2	3	4	5	6
Calibration samples	A	30	40	50	60	70	80
	B	40	60	80	30	50	70
	C	50	80	40	70	30	60
Test samples	A	60	30	70	40	80	50
	B	70	50	30	80	60	40
	C	80	70	60	50	40	30

2.1 Method example analysis based on support vector machine

For the convenience of discussion, three-component (A, B, C) spectral system data simulated with computer is used for example analysis. Different peak height, peak width and peak position are set up for different components; and the unit spectrum of three components are obtained with gaussian function as the integral absorptivity of each component, thus the measuring sample consisting of 12 different concentration is designed with the uniform design method, 6 of which as the correction sample set, and the other 6 as the inspection sample set; the concentration is shown in Table 1; the absorbancy curve of each sample is obtained by adding the gaussian white noise and multiplied by relevant interference factor, which is considered as the original data of simulation analysis. See the single component spectrum of A, B and C in Figure 1; see the de-noise effect of wavelet transform in Figure 2.

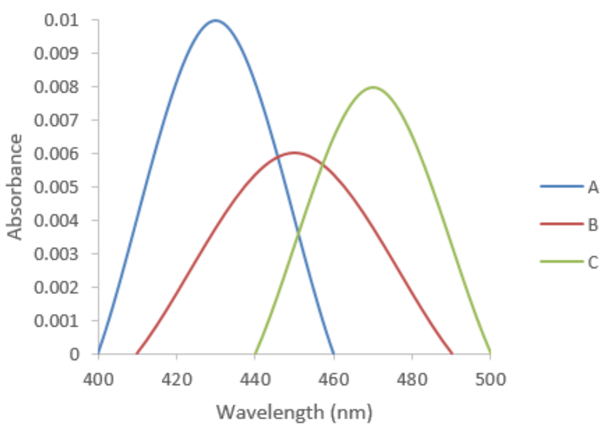

Figure 1: Single component spectrum (A, B, C)

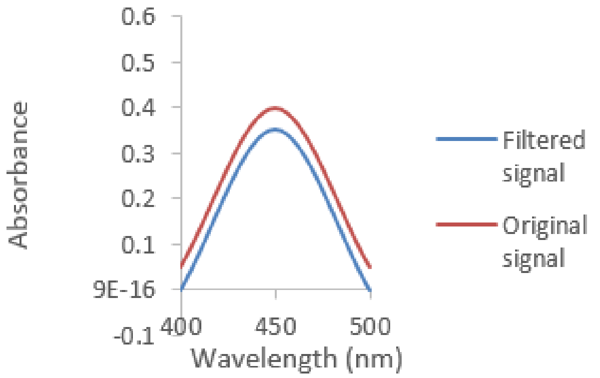

Figure 2: Denoise with wavelet transform

2.2 Example analysis of wavelength selection

The final objective of wavelength selection is to improve the prediction capability of the model. The prediction residuals are the most basic performance evaluation indicators for the prediction capability of evaluation model (Ibarrondo et al., 2016). In case the complexity of the calculation can be reduced and the satisfactory solution can be found out through calculation, the prediction residuals square of the inspection sample set is considered as the fitness function (Jain et al., 2014). As the prediction residuals are only related to the model established, but also related to the concentration of each detailed sample; in order to eliminate such influence, the ratio between prediction residuals and sample concentration is the most basic fitness function of unit structure f($x_{k,f}$) so as to replace the prediction residual quadratic sum, see the details as follows:

$$f(\hat{x}_{k,f}) = \frac{100}{nm}\sum_{k=1}^{n}\sum_{f=1}^{m}\left|\frac{(\hat{x}_{k,f} \quad x_{k,f})}{x_{k,f}}\right| \tag{1}$$

Where, n is the number of samples; m is the number of components; x_{kf} means the real concentration of No. k samples and No. f component; x_{kf} means the prediction concentration of No. k sample and No. f component. The wavelength selection algorithm is always used together with certain prediction methods, such as the genetic algorithm and partial least squares (PLS) or principal components regression (PCR) or other multiple regression methods. Theoretically, the wavelength selection algorithm can be used by combining most prediction methods.

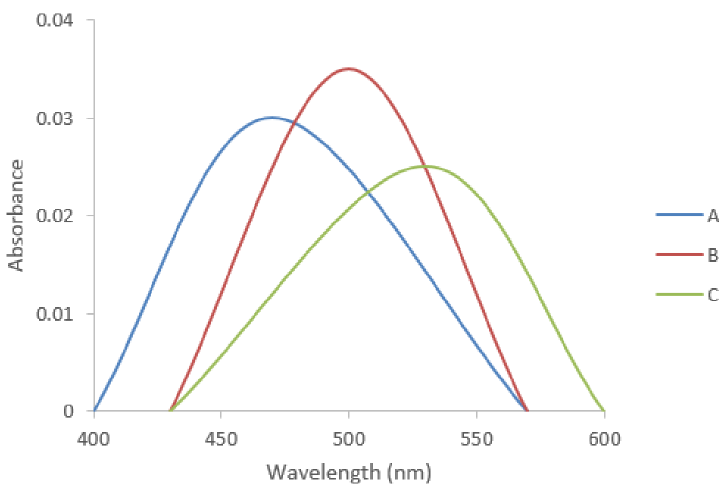

Figure 3: Single component spectrum (A, B, C)

As for actual spectral data, one kind of which is that different measuring points are subject to the interference of different white noise of different strength. The other kind is that measuring wavelength pints are subject to the influence of uniform white noise, however, different nonlinear factors exist in different wavelength area. Relevant experiment data can be obtained through computer simulation in both cases. If the multiple-component solution sample containing A, B and C component is to be analysed, then the single-component spectrum of A, B and C is shown in Figure 3.

3. Design and analysis of spectral recognition system

The spectral signal is the research object of spectral recognition system, which is used to judge and appraise the property of substance by comparing the difference between spectrums (Jogi et al., 2013). As the substance is of many varieties, and the spectrum of different substances, small differences also exist in the same substances (herein refers to mixture such as medical materials and tobacco etc.); how to identify such spectrums accurately is the basis for the design of spectral recognition system (Kielmann et al., 2014). In addition, as for many industries, the spectrum required to be identified is not fixed, but increased continuously. In case of the origin judgment or level judgment process of some farming products, this requirement is obvious (Kong and Notingher, 2016). Therefore, good expansibility is required, and the capability of adapting the continuous expansion demand of the system must be considered in the design process of spectral recognition system.

3.1 Feature extraction of spectral signals

As for mode identification, feature is the key indicator for distinguishing the sign things from other things; generally speaking, feature extraction is the premises for mode identification, which is also applicable to the spectral recognition system; common features include the time domain characters, frequency domain features and wavelet domain characters etc (Kourti, 2015). The detailed discussion about the spectral signal in time domain, frequency domain and wavelet domain etc. are presented.

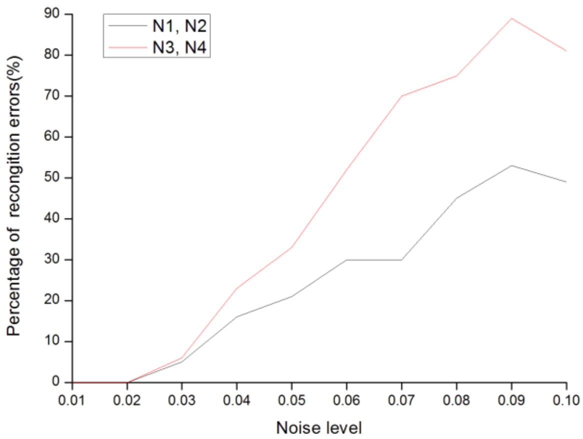

Figure 4: The relationship of recognition error and noise of N1, N2 and N3, N4

The time domain feature of spectral signal: the time domain feature of spectral signal is the most basic feature. The spectral signal extracted generally includes the wave crest, wave trough and inflection point etc. (Lackner et al., 2014). As for many signals, the wave crest, wave trough and inflection point etc. can be compared directly so as to obtain the judgement result quickly. The description hereunder is made with wave crest as the example, the similar method is also applied to the wave trough and inflection point.

Table 2: Table about peaks of four spectrums

Wave size sorting	1	2	3	4	5
Spectrum 1(nm)	235	350	700	550	450
Spectrum 2(nm)	700	550	350	450	235
Spectrum 3(nm)	235	350	700	550	450
Spectrum 4(nm)	235	350	700	550	450

Table 2 is the wave crest of four spectrums, from which the difference of wave crest of spectrum 1 and spectrum 2 is obvious, although the size and sequence of their wave crests are different; therefore, we can separate them rapidly.

3.2 System design and analysis

The essence of spectral recognition is to find out and establish the mapping reflection between the input spectrum data space and the output spectrum type space. As for the handling of two problems, the support vector machine is the most effective method; according to current report, the neural network is the most commonly used and successfully applied method; and the neutral network is of advantages lacked in general linear system, which can conquer the limitation of many traditional mode identification methods; therefore, the neutral network method is considered to be used for the design of spectral recognition system (Lei et al., 2016). A spectral database consisting of four spectrums is designed hereunder, and the entire process of spectral recognition system is introduced by judging if the unknow spectrum belongs to one of these four spectrums. The wave crest position is the feature of presorting in the spectral recognition system; and the wavelet character is considered as the input feature of neutral network. Four spectrums include N1, N2, N3 and N4.

See the relationship between the false recognition rate and signa level of the probabilistic neural network of N1, N2, N3 and N4 in Figure 4; as for N1 and N2, when the noise level is 0.04, the false recognition rate is 16%. As for N3 and N4, when the noise level is 0.04, the false recognition rate is 25%. Theoretically, the false recognition rate may be higher in case of the noise level is larger; and the figure shows such overall trend; however, some fluctuations exist due to the insufficient simulation times; in addition, the setting of neutral network parameters may be one of the reason. As for spectrometer, the noise is considered as large if the noise level is 0.04.

4. Conclusions

This paper deeply studies multi-component measurement of spectral signals, with the aim of efficiency and practicability, analyzes and discusses in details from experimental design to algorithm selection, and puts forward the combined algorithm and strategy based on uniform design, wavelet transform and support vector machine to solve nonlinear correction problems in multi-component spectra measurement. It also discusses the wavelength selection during quantitative analysis of spectral signals and puts forward the segmented wavelength selection method based on particle swarm optimization algorithm to solve the subjective randomness for wavelength selection during quantitative analysis and compliexity and slow convergence of the existing methods. In addition, it also deeply explores the identification of spectral signals, correspondingly analyzes and discusses the basic spectral recognition method and feature extraction of spectral signals, and puts forward the method for building a spectral recognition frame through multiple features and neural networks, so as to quickly and correctly recognize the spectral signals.

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