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Application of Adaptive Iteratively Reweighted Penalized Least Squares Baseline Correction in Oil Spectrometer

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Abstract: *In order to solve the problem of baseline drift caused by spectral lines of oil spectrometer, an adaptive niteratively reweighted penalized least squares method is proposed to correct the baseline. The oil spectrometer of Kunshan Soohow Instrument Technology Co. Ltd. was used to measure the contents of various elements in the standard oil with four concentrations of 0ppm, 10ppm, 30ppm and 50ppm. The spectral line data collected by the first CCD was processed, and a good baseline correction effect was obtained.*

Keywords: *Adaptive iterative weighting, Least square method, Baseline correction, Oil spectrometer*

1. Introduction

In order to reduce the friction loss of mechanical equipment, lifting equipment use safety and service life of the oil is widely used in mechanical equipment lubrication protection, but with the increase of using time or mechanical design or installation itself on the tiny mismatch defects, such as mechanical equipment running process still produces a small amount of different degree of wear and tear. These wear will produce metal or non-metal abrasive particles in the lubrication system of the equipment, which will affect the lubrication effect of the oil in the process of repeated use. More serious, it will lead to accidents or even complete damage of the equipment, and the economic loss will be inestimable[1]. Therefore, the routine component detection of multi-element abrasive particles in lubricating oil is of great significance. Such routine and accurate detection can not only routinely detect the health condition of mechanical equipment, but also provide early warning before the occurrence of equipment wear fault, effectively guaranteeing the normal operation of equipment[2]. Lubricating oil is composed of fewer elements, but its structural state is more complex and exists in the form of organic matter. The elements measured are mainly the lubricating oil in the operation process due to equipment wear and tear into the oil. In the specified time, as long as the wear quantity does not exceed the allowable value, it is considered normal wear, normal wear rate can be used to predict and determine the life expectancy of the machine, performance ratio and other indicators; The abnormal wear rate indicates a potential trouble with the machine. Through the analysis of the lubricating oil sample of check out in the lubrication system, according to the result of the metal elements concentration data can infer the metal working parts wear degree, so as to detect the cause of equipment failure or avoid device and a fatal failure due to abnormal wear, oil spectrum analysis technology is based on the fact. By analyzing the contents of these wear elements (Fe, Al, Cu, Ni, Cr, Sn, Pb, Ag, Cd, Mn, Ti, V) [3].

Penalty least squares is a flexible smoothing method, which mainly includes two aspects: the smoothing of the signal by penal least squares and the penal least squares algorithm that transforms the penal process into a baseline estimation by adaptive iteration[4]. This method is easy to operate without any user intervention and initial information. Based on the penalized least squares, the sum of squares for error (SSE) weight between the fitting baseline and the original signal is adjusted adaptively in the iterative process. The SSE weight is obtained by the difference between the fitting baseline and the original signal before the adaptive use. This method can quickly and flexibly deduct the baseline of irregular changes[5]. This baseline processing method has low data requirements, convenient and fast processing process, and is very suitable for large-scale sample sets.

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2. Algorithm principle

The experiment uses MATLAB software to adopt adaptive iteratively Reweighted Penalized least-squares (airPLS) can eliminate the spectral background in batches from the oil sample spectra[6-8]. adaptive iteratively Reweighted Penalized least-squares is a baseline correction method recently proposed by Liang Yizeng et al.[9].

The method is in the punishment, on the basis of least square by adaptively adjusting in the process of iterative fitting between baseline and original signal SSE the weight of residual sum of squares), quickly and flexibly to find irregular change of baseline and deduction[10].

2.1 Punish the least square method

Penalized least-squares algorithm was first proposed to filter. But in recent years, it has been extended to the background subtraction of spectral signals. Here's how it works.

Suppose *x* is the vector of the analysis signal and *z* is the fitting vector with length m. The fidelity of *z* against *x* can be expressed by the population variance between them:

$$F=\sum_{i=1}^{m}(x_i-z_i)^2 \tag{1}$$

The roughness of fitted data *z* can be expressed by the sum of squares of its difference:

$$R=\sum_{i=2}^{m}(z_i-z_{i-1})^2 \tag{2}$$

The balance between precision and roughness can be expressed by *Q*:

$$Q=F+\lambda R=\sum_{i=1}^{m}(x_i-z_i)^2+\lambda\sum_{j=2}^{m}(z_j-z_{j-1})^2 \tag{3}$$

2.2 Adaptive iteration weighting

The adaptive iterative reweighting method is similar to the Weighted Least Square and Iterative Penalty Least Square processes, but the difference lies in the weight calculation method and the addition of penalty terms to control the smoothness of the fitting background. The optimized objective function is:

$$Q=w^tF^t+\lambda R^t=\sum_{i=1}^{m}w^t(x_i-z_i^t)^2+\lambda\sum_{j=2}^{m}(z_j^t-z_{j-1}^t)^2 \tag{4}$$

Each iteration *w* can be obtained as follows:

$$w^t=\begin{cases}0 & x_i\ge z_i^{t-1}\\ e^{\frac{t(x_i-z_i^{t-1})}{\left|d^t\right|}} & x_i<z_i^{t-1}\end{cases} \tag{5}$$

The vector d^t contains all elements whose difference between the original Raman spectrum *(X)* and the fitting vector Z_i^{t-1} in the iteration process is negative. In the first *t-1* iteration, the fitting vector is a candidate for background estimation. If the current calculation is greater than one candidate of this background estimate, it is considered to be in the position of the peak. At this point, the weight is reset to 0 so that it does not affect the next iteration. In the process of air-PLS algorithm, iteration and reweighting are carried out automatically continuously, so that the data points in the peak position can be gradually eliminated and the background points can be retained in the weight vector. The number of iterations or some convergence condition can be set to terminate the iteration.

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3. Experiment

3.1 Experimental Instruments

The experiment was carried out using OIL8000 oil spectrometer (Kunshan Soohow) as shown in Figure 1.

Optical system: high-performance holographic diffraction grating, grating lines 2700 /mm, focal length 500 mm; Multi-block high performance CCD detector system; Each CCD has 3,648 pixels, and there are eight CCDs in total.

Sspark power supply: oscillating arc discharge control, electronic acquisition and data readout system; The electronic system has the function of multi-channel integration and data collection system controlled by microprocessor. High speed 16-bit analog-to-digital converter.

Fig.1.OIL8000 oil spectrometer

3.2 Experimental samples

Petroleum ether: analytical pure;

Standard oil: 0×10^{-6}, 10×10^{-6}, 30×10^{-6}, 50×10^{-6}PPM, respectively.

The standard oil is shown in Figure 2.

Fig.2.Standard oil

3.3 Experimental process

In the best working condition of the instrument and the selected working conditions, a series of standard oil samples are excited, and the working curve is drawn, and then the analysis samples are excited under the same working conditions. The spectra of the first CCD at four concentrations were collected, and the spectra of the four concentrations were used as adaptive iterative weighted penalized least square method to correct the baseline.

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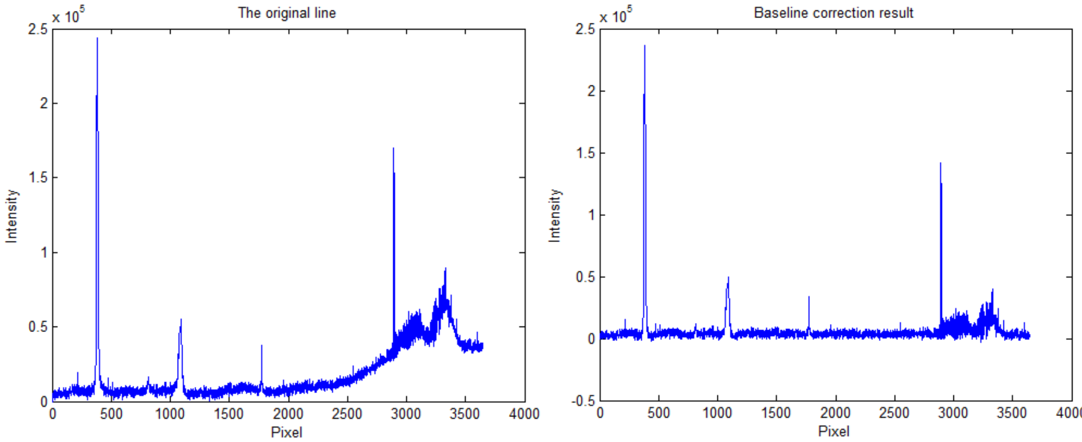
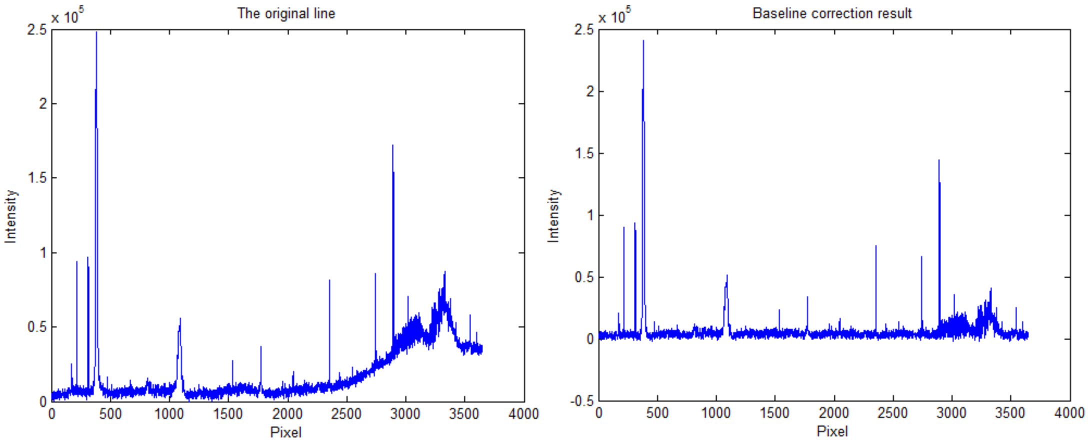
4. Experimental results and analysis

The experiment uses MATLAB software to adopt adaptive iteratively penalized least square method Reweighted Penalized least-squares (airPLS) is used to deduct the baseline batch from the spectra collected by the first CDD of oil samples with concentrations of 0×10^{-6}, 10×10^{-6}, 30×10^{-6}, and 50×10^{-6} PPM. The effect before and after baseline correction is shown in Fig. 3-6.



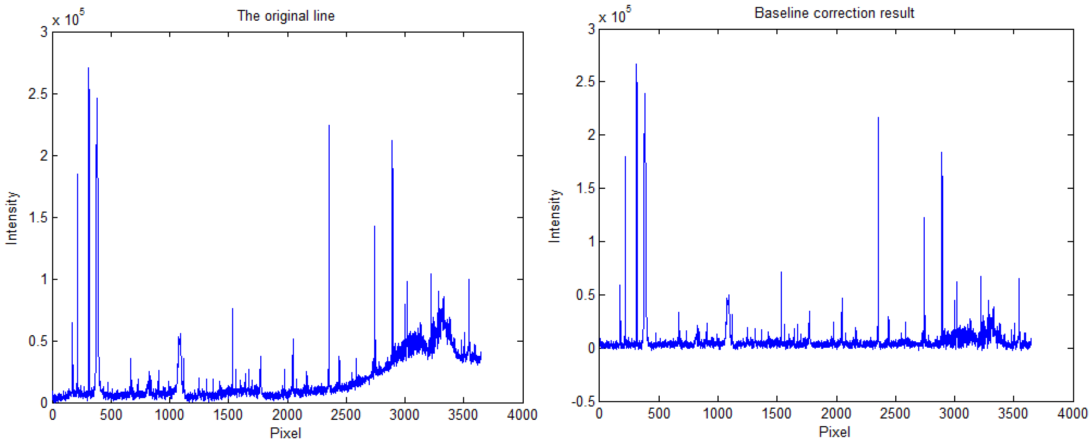
(a) Spectral lines before baseline correction (b) Spectral lines after baseline correction

Fig.3. Standard oil spectral line with a concentration of 0ppm



(a) Spectral lines before baseline correction (b) Spectral lines after baseline correction

Fig.4. Standard oil spectral line with a concentration of 10ppm



(a) Spectral lines before baseline correction (b) Spectral lines after baseline correction

Fig.5. Standard oil spectral line with a concentration of 30ppm

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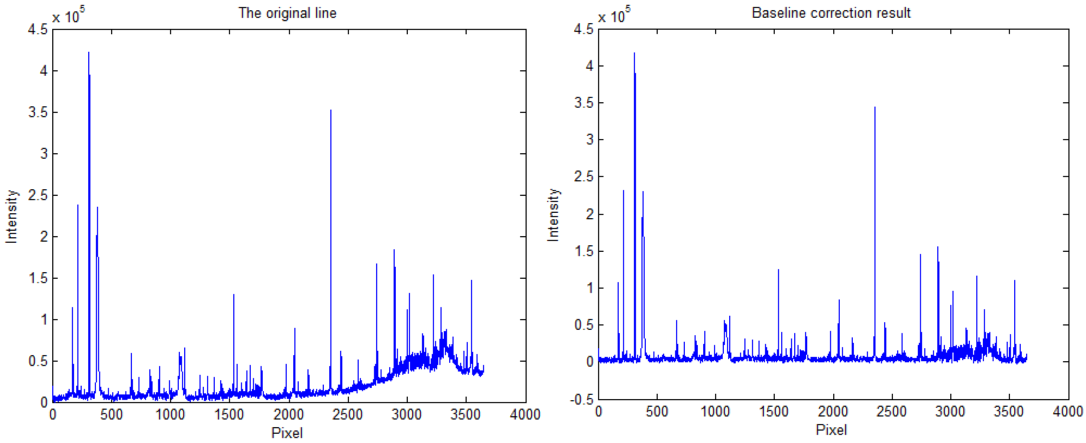

(a) Spectral lines before baseline correction *(b) Spectral lines after baseline correction*

Fig.6. Standard oil spectral line with a concentration of 40ppm

Through careful observation of Fig. 3-6, it can be seen that the baseline of the spectral lines of each concentration is corrected to the vicinity of 0, reaching a relatively stable state. Such prominent baseline correction effect plays a role in improving the measurement accuracy in the subsequent transition from spectral peak intensity to element content.

5. Conclusions

In this paper, the adaptive iterative weighted penalized least square method is used to calibrate the spectra obtained by oil spectrometer. The experimental results show that the adaptive iterative weighted penalized least square method, as an advanced and simplified baseline correction algorithm, has a good application prospect for the spectral processing of oil spectrometer (i.e. rotating disc atomic emission spectrometer).

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