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Research on ultraviolet-visible absorption spectrum preprocessing for water quality contamination detection

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ABSTRACT

The contaminant detection in water is important to secure public health against potentially harmful substances. As a noninvasive detection technique, ultraviolet-visible (UV-Vis) spectroscopy is studied and widely applied in detecting water contamination. However, current methods for contamination detection reveal the defects of noise sensitivity and data redundancy. In this study, de-noising and dimensionality reduction of UV-Vis absorption spectrum are focused on. With regards to de-noising, the influence of various discrete wavelet transforms families, decomposition levels and threshold methods on UV-Vis absorption spectrum de-noising are analyzed and discussed in detail. Concerning dimensionality reduction, the principal component analysis (PCA) is utilized. The performance of de-noising and dimensionality reduction is assessed by signal-to-noise ratio (SNR) and normalized reconstruction error (ε_{norm}), respectively. Results from experiments and analysis reveal the decomposition level and wavelet transforms families are the most significant parameters influencing the de-noising algorithm efficiency. Moreover, using sym5 at five level decomposition with hard threshold method had the best effect for UV-Vis absorption spectrum de-noising. Besides, PCA can project UV-Vis absorption spectrum to a much lower dimension but representative data space.

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1. Introduction

Water is a fundamental resource for humanity existence, which is essential in production process and our daily life. However, because of environmental destruction, water pollution has become a serious problem threatening the survival of human beings, plants and animals. Thus, a real-time detection system for water quality is of great need to secure public health against potentially harmful substances.

As a continuous on-line detection method, UV-Vis spectroscopy is increasingly applied for detecting water contamination. Therefore, many scholars in home and abroad have done many researches in this area. However, most of the present studies on water quality detection are based on pure spectrum analysis [1]. For UV-Vis spectroscopy, absorption spectrums are often disturbed by various factors, including power frequency interference from light sources, variability in hydraulics, suspended matters, and contaminants [2]. These various noise makes water quality contamination detection based on UV-Vis spectroscopy difficult or even impossible. On the other hand, the UV-Vis spectrum of each water sample is a high-dimensional vector. In most cases, high-dimensional vectors arise many difficulties and challenges for data processing [2]. A UV-Vis absorption spectrum with strong noise is shown as Fig. 1.

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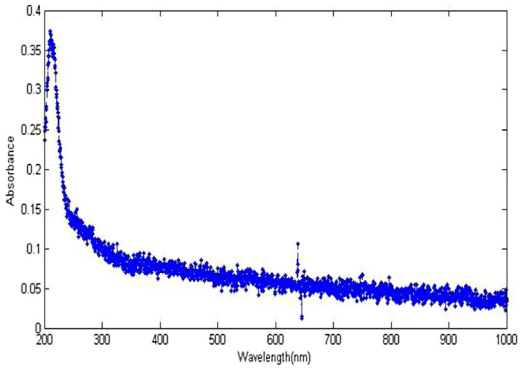

Fig. 1. UV–vis absorption spectrum of a water sample with strong noise.

Table 1
Some researches on signal preprocessing.

Researchers	Method	Conclusion
Gai et al. [9]	Combination color monogenic wavelet tranform (CMWT)	Proposed algorithm can effectively remove noise from image by prior knowledge of noise characteristics
Ali et al. [8]	Discrete Fourier Transform (DFT)	Four levels of decomposition using DWT can remove the noise from heart sound signals effectively
Koga et al. [23]	Principal component analysis (PCA)	The first principal component of Itokawa surface spectra can reflect space weathering
Vazquez et al. [24]	Blind source separation (BSS) and wavelet denoising (WD)	The method successfully rejected a good percentage of artefacts and noise from scalp electroencephalogram recordings (EEG)
Kong et al. [10]	DBN wavelet transform denoising	Under this denoising method, it is feasible to employ near-infrared spectroscopy for rapid detection of straw components

Consequently, in this study, we propose a preprocessing method based on Discrete wavelet transform (DWT) and PCA to effectively eliminate the noise from UV-Vis absorption spectrum and realize dimensionality reduction. In order to achieve this goal, the influence of various discrete wavelet transforms families, decomposition levels and threshold methods on UV-Vis absorption spectrum de-noising are analyzed and discussed in detail. With regards to dimensionality reduction, PCA is applied to realize dimensionality reduction. The performance of de-noising and dimensionality reduction is assessed by signal-to-noise ratio (SNR) and normalized reconstruction error (ε_{norm}), respectively.

In next section, the related literatures are reviewed. In section 3, theoretical background on the tools used is given. In section 4, the methodology used is presented. In section 5, the experimental results are discussed. In section 6, the conclusion about this study is given.

2. Literature review

Many researches are reported to improve the data quality and detection precision of water contamination. A widely used method is using multiple conventional water quality parameters and analyzing the mapping relationship between the parameters and water contamination. Liu et al. [3] established an Early Warning System (EWS) by exploring the correlative relationships between multiple types of conventional water quality sensors. This EWS can provide a fast and accurate way to differentiate contamination events from normal variations. Yang et al. [4] explored a real-time event adaptive detection, identification and warning method based on enhancing contaminant signals and classification, which improved the performance of contamination detection. However, the measure of these conventional water quality parameters needs long-time and high cost, due to whose measurements are mainly obtained through wet chemistry.

In recent years, one widely accepted method for contamination detection is based on UV-Vis spectroscopy. This method has the characteristic of easy measurability, low-cost and continual detecting. Due to this, the technique has already been attempted and studied as an alternative method in this application. Zhu et al. [5] successfully applied UV-Vis spectroscopy coupled with principal component analysis (PCA) and hierarchical cluster analysis (HCA) to characterize dissolved organic matter (DOM). This method can characterize DOM fractions of lakes, which has been proved in Dongjianghu Lake. Huang et al. [6] applied approximate entropy (ApEn) to detect water quality contamination events. This method is not sensitive to signal disturbance and can make a distinction between normal and abnormal signals. Although many studies have been done for contamination detection based on UV-Vis spectroscopy, yet signal disturbance has always been a problem affecting measurement accuracy.

For signal preprocessing, DWT and PCA [7] are widely used and quite efficient, because DWT is able to analyze signal at various resolutions by different kinds of wavelet families [8–11] and PCA can overcome the redundancy and multi-collinearity. As shown in Table 1, some preprocessing studies have been listed. However, there are few studies on the application of DWT

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