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Analysis of skin influence in identification of heroin using Singular Value Decomposition

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Abstract

In this paper, the influence of skin in energy-dispersive X-ray diffraction (EDXRD) spectrum of heroin was studied using singular value decomposition (SVD). The spectra of pure heroin, skin and heroin covered by skin were organized as matrices for SVD after truncation and smoothing. It was demonstrated that the two largest singular values and their corresponding left and right singular vectors of each matrix could reconstruct the matrix in the permissible error and contained enough information of the matrix. We extracted the two largest singular values of each matrix as two dimensions of the feature point of the corresponding spectrum. The feature points of different samples were clustered and a linear relationship was proved to be between and movement of feature point and thickness of component of skin, such as fat and muscle. This indicated that the method of SVD may be suitable for identification of heroin covered by skin.

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Keywords: heroin identification; singular value decomposition; energy-dispersive X-ray scattering.

1. Introduction

Drug smuggling has been an important criminal activity all over the world for many years. Recently, it has become a main approach that drug is packaged in human body for trafficking. In this situation, how to detect drug covered by skin has become an important research topic. Among some different techniques for detection of drug, energy dispersive X-ray diffraction (EDXRD) has been proved to be a suitable approach with several particular advantages, such as non-destructive, non-invasive, low-cost, high-resolution and etc.[1-3]

Here, heroin is chosen as the representation of drugs. The EDXRD spectrum of heroin in our experiment is constructed of 1024 data according to the 1024 channels of the detector. And the 1024 channels refer to the energy of the incident X-ray. However, after packed in human body, the skin will not only attenuate the energy of the X-ray, but also infect the spectrum due to elastic scattering and inelastic scattering.

In this paper, our work mainly focus on the analysis of skin influence to the spectrum of heroin. The feature of the EDXRD spectrum is extracted through SVD, which is a popular mathematical method used in multi-dimensional data analysis. Because the muscle and fat of pig is very similar to the human's, the combination of them in different proportion is used instead of human skin.

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2. Methods and experiment

2.1 EDXRD and experimental system

EDXRD utilizes the X-ray photons coherently scattered at small angles (less than 10°) to the incident beam. At these angles coherent scatter dominates over coherent, or Compton scatter [1]. The coherently scattered photons interfere with each other producing diffraction peaks according to Bragg's law;

$$n\lambda = 2d \sin(\theta/2) \quad (1)$$

Where λ is the wavelength of the photon, n an integer greater than zero, d the spacing between scattering centres and θ the angle through which the photon is scattered.

In practice we measure the scattering intensity from a material as a function of either:

- The angle of coherent scatter at a fixed X-ray photon energy;
- The energy of coherent scatter at a fixed scattering angle.

Method a) is an extension of the conventional small scale X-ray diffraction chemical analysis technique and requires a monochromatic X-ray source and an imaging photon counting detector to record the scattering intensity across the desired angular range. Method b) requires a high purity germanium energy dispersive X-ray detector and a polychromatic X-ray source. [2]

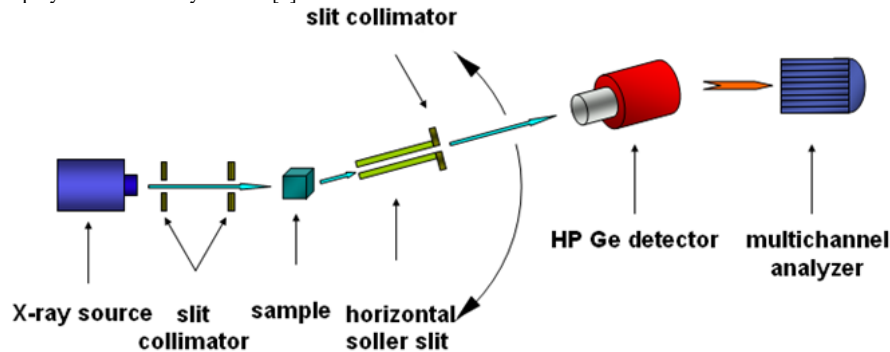


Fig.1. Structural representation of EDXRS

The experiments are performed using the home-built energy-scanning diffractometer in the Institute of Intelligent Machines, Chinese Academy of Sciences, which consists of X-ray source, optical system, detection systems and mechanical control system as shown in Figure 1. This instrument has been introduced by Bai Sun in details. [4]

2.2 Singular value decomposition

SVD is a technique commonly used in the analysis of spectroscopic data that both acts as a noise filter and reduces the dimensionality of subsequent least-squares fits. [5] It also has been successfully used in some other areas such as the analysis of molecular dynamics simulations [6] and the temporal variation of genome-wide expression [7].

The existence of the SVD of a general rectangular matrix has been known for over fifty years. For an $m \times n$ matrix A with real elements ($m \geq n$), the SVD is defined by:

$$A = USV^T \quad (2)$$

Where U is an $m \times n$ matrix having the property that $U^T U = I_n$, where I_n is the $n \times n$ identity matrix, V is an $n \times n$ matrix such that $V^T V = I_n$, and S is a diagonal $n \times n$ matrix of nonnegative elements. The diagonal elements of S are called the singular values of A and will be denoted by $s_k, k \in \{1, 2, \dots, n\}$. The columns of U and V are called the left and right singular vectors of A , respectively. The singular values may be ordered (along with the corresponding columns of U and V) so that $s_1 \geq s_2 \geq \dots \geq s_n \geq 0$. With this ordering, the largest index r such that

$s_r > 0$ is the rank of A , and the first r columns of U comprise an orthonormal basis of the space spanned by the columns of A . An important property of the SVD is that for all $k \leq s$, the first k columns of U , along with the corresponding columns of V and rows and columns of S , provide the best least-squares approximation to the matrix A having a rank of k [8]. The singular values of a matrix also have many other significant properties such as stability, linearity and rotation invariance.

2.3 Data process based on SVD

The spectrum of pure heroin or heroin covered by skins from EDXRD consists of 1024 data. EDXRD spectra of pure heroin, skin and heroin covered by heroin are given in Figure 2 as example. The x -coordinate represents the 1024 channels of the multi-channel analyzer, equivalent to the energy spectrum of 0–50 keV; the y -coordinate represents the number of photons detected by different channels. Peaks near 10 keV in the energy-coordinate result from fluorescence metallic target, while the profiles after fluorescence peaks originate from heroin sample.

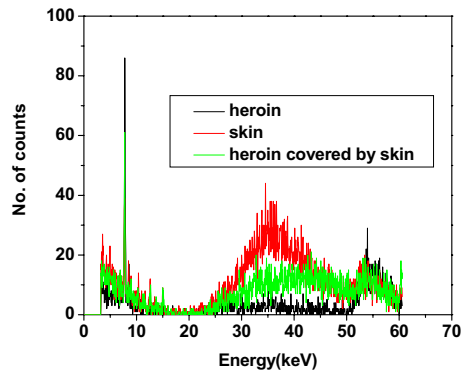


Fig.2. EDXRD spectra of pure heroin, skin and heroin covered by skin

These spectra have to be processed through three steps for the analysis of SVD. The first step is truncation which refers to reduction of the size of spectrum data. As mentioned above, the peaks near 10 keV result from fluorescence metallic target which are useless and adverse for the analysis and computation. Therefore, we select 512 data between 251 and 762 in channels (about 14.88 keV to 45.08 keV in energy-coordinate). The second step is the organization of the matrices required by SVD from the preprocessed spectra. We continuously cut each of the preprocessed spectra, which has 512 data, into 32 sections of the same length and take each section as a column to construct a 16×32 matrix. This matrix is unique to particular sample and contains all the information of the spectrum. The third step is the calculation of SVD of the data matrix. Then we get the two biggest singular values of the matrix as the feature point of the sample.

3. Results and discussion

In this paper, 13 groups of samples were prepared, each group was measured eight times. The 1st group of samples is pure heroin; the 2nd and 3rd groups were skin (muscle and fat) of different thicknesses, while the proportion of muscle and fat was 1:1, and the thicknesses of skin were separately 40, 60 mm; the 4th to 7th groups were heroin covered by muscle of 10 mm and fat of different thickness, and the thicknesses of fat were separately 10, 20, 30, 40 mm; the 8th to 10th groups were heroin covered by fat of 10 mm and muscle of different thickness, and the thicknesses of fat were separately 20, 30, 40 mm; the 11th and 12th groups were heroin covered by the skin which are the same with 2nd and 3rd groups. We got feature points of these spectra through the process mentioned in section 2.3. The feature point is a two-dimensional point whose first dimension is singular value 1 while the second one is the singular value 2.

Analysis result of spectra of heroin covered by skins is shown in Figure 3. Three conclusions can be reached from this figure. Firstly, eight feature points of each sample focuses on a particular area which is far away from areas of other samples. Secondly, when the thickness of muscle fixes at 10 mm, the singular values especially the first one grow with the increasing thicknesses of fat. An approximate linear relationship exist between the singular value 1 and the thickness of fat. Thirdly, after the thickness of fat is fixed at 10 mm, an approximate linear relationship can also be found between the singular value 1 and the thickness of muscle.

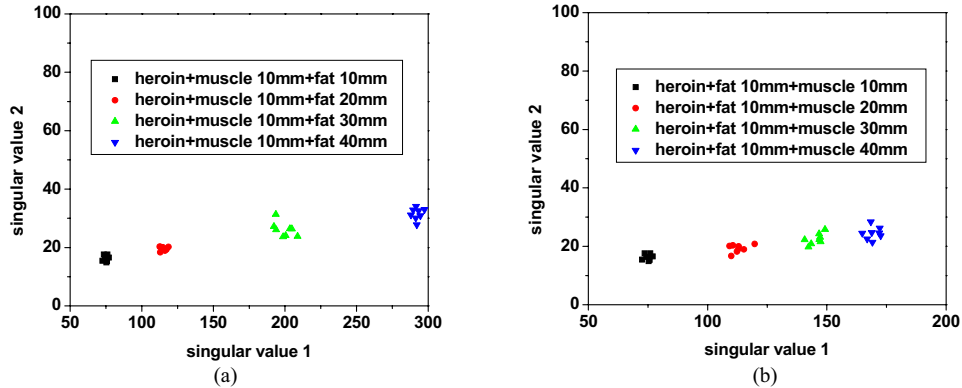


Fig.3. Score plot of singular value 1 against singular value 2: (a)the thickness of muscle fixes at 10 mm and thicknesses of fat is 10, 20, 30, 40 mm; (b) the thickness of fat fixes at 10 mm and thicknesses of muscle is 10, 20, 30, 40 mm.

In the identification of heroin covered by skin (packaged in human body), the main work is to distinguish spectra of normal human body and the human body packaging heroin. In figure 4, the feature points of pure heroin, skin of different thickness and heroin covered by the same skin are shown. It implies that the feature points of pure heroin, skin and heroin covered by the same skin are separately clustered well. It is easy for us to distinguish if the skin covers heroin or not. This is very meaningful for the application of identifying the heroin packaged in human body.

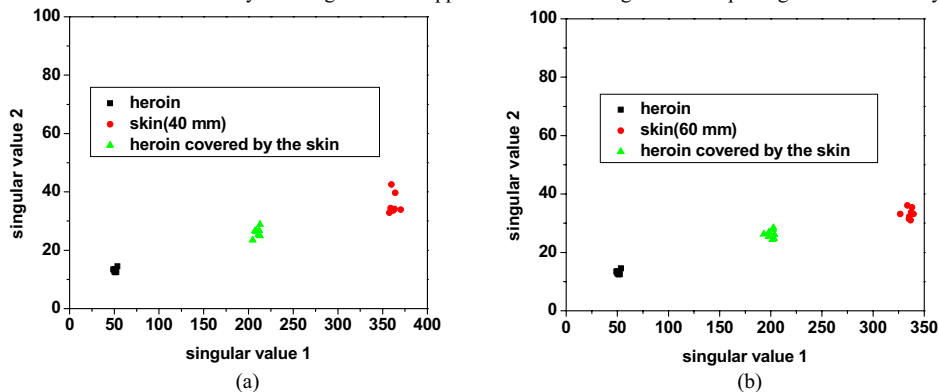


Fig.4. Score plot of singular value 1 against singular value 2: (a) feature points of pure heroin, skin with thickness of 40 mm(fat 20 mm, muscle 20 mm) and heroin covered by the skin; (b) feature points of pure heroin, skin with thickness of 60 mm(fat 30 mm, muscle 30 mm) and heroin covered by the skin.

Conclusions

The method based on SVD has been used to analyse the skin influence in identification of heroin. In the space of singular values, feature points of samples of different compositions located different areas. After the thickness of fat/muscle is fixed, the singular value 1 of the heroin covered by skin grows with the increasing thickness of muscle/fat. The spectra of sample of skin and the same skin covering heroin is analysed in comparison. The feature points of skin covering heroin is clustered and far away the skin which doesn't cover heroin. It imply that this method is hopefully suitable for identifying the heroin packaged in human body.

Acknowledgements

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