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RESEARCH ARTICLE

2-D Image Localization in Hyperspectral Image Analysis of Pharmaceutical Materials

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Abstract
Introduction Discriminant analysis (DA) is often used in hyperspectral image processing to classify multiple components on a sample matrix.
Methods In DA, a customized threshold is typically applied in a univariate domain, such as a projected score or predicted concentration value, in order to differentiate multiple components. However, determination of an appropriate threshold is subjective and influenced by both material- and user-dependent factors. Moreover, the potential of different thresholds to yield conflicting results poses a significant concern and challenge for pharmaceutical scientists.
Results The photon radial diffusion among adjacent pixels in a near-infrared chemical image has been documented in literature to be a significant contributor to the challenges associated with the threshold-dependent image analysis. Therefore, in this study, a 2-D image of a score scatter plot was developed to visualize and identify the localization of individual components in a sample matrix, instead of a univariate projected score.
Conclusions An NIR chemical imaging dataset of cylindrical compacts of binary mixtures, including microcrystalline cellulose and different sized polystyrene microspheres, was used to demonstrate the efficiency of the method. The application of the method on hyperspectral image analysis on pharmaceutical multi-component systems was also presented.

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Keywords Hyperspectral imaging · 2-D image localization · Photon diffusion · 2-D image of a scatter plot · Discriminant analysis

Introduction

The number of qualitative and quantitative applications of chemical imaging in the field of pharmaceutical analysis has increased dramatically in the past 5 years. The main reason is its capability to capture the spatial distribution of both physical and chemical properties of a sample matrix using the pixel-by-pixel information. With more attention being paid to the potential of chemical imaging, researchers are realizing the importance of photon diffusion and its corresponding spatial dispersion in chemical images. These phenomena have been reported in both near-infrared (NIR) [1] and Raman chemical images [2]. Because of the photon diffusion along both the depth and radial directions, spatial information existing outside of an observed pixel is detected within the pixel. Thus, spatial dispersions are observed, especially at the edge of a substance in a chemical image.

Partial least square-discriminant analysis (PLS-DA) has been used to classify the contents of pixels in routine chemical image analysis. The general procedure involves three steps. The first step is to establish a PLS-DA model based on the pure component spectra collected from pure component images. The second step is to use the PLS-DA model to generate a histogram of predicted concentration values for each component of interest in a sample image. The third step is to select a threshold on the histogram that differentiates the individual components. Pixels showing a predicted concentration larger than the threshold are classified as the component of interest, while the remaining