

MEETING ABSTRACT

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Spatial segmentation and feature selection for desig imaging mass spectrometry data with spatially-aware sparse clustering

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Background

Recent experimental advances in matrix-assisted laser desorption/ionization (MALDI) and desorption electrospray ionization (DESI) have demonstrated the usefulness of these technologies in the molecular imaging of biological samples. However, development of computational methods for the statistical interpretation and analysis of the chemical differences present in the distinct regions of these samples is still a major challenge. In this poster, we propose statistically-minded methods and computational tools for analyzing DESI imaging experiments. Specifically, we present techniques for signal processing and unsupervised multivariate image segmentation, which are also applicable to other imaging mass spectrometry (IMS) methods such as MALDI.

Method

Signal processing of DESI spectra typically involves binning to reduce dimensionality, but this is inefficient for downstream analysis as it retains empty regions of the mass spectrum. In our proposed processing step, we apply a novel peak picking algorithm based on windowed smoothing splines that allows adaptive resolution based on spectral profile. With this approach, peaks are aligned using a recursive dynamic programming algorithm which accounts for the heterogeneous nature of IMS data by making pairwise alignments between pixels based on their proximity. Peaks are then normalized using total ion count.

In order to segment the sample into sub-regions of homogeneous chemical composition in MALDI images,

Alexandrov & Kobarg [1] proposed two efficient spatially-aware clustering techniques. We demonstrate that these approaches are also useful for DESI. Moreover, we extend one of these clustering methods using statistical regularization techniques that enable simultaneous feature selection of structurally-important peaks and facilitate interpretation.

Conclusions

We evaluate the performance of the proposed methods in two applications. First, in a non-biological application of DESI-imaging, we recreate a painting from the clustering of its DESI mass spectra (Figure 1). Since the visual content of the painting is known, it can be used as a gold standard to evaluate the performance of these methods. In the second application, we present the spatial segmentation of a fetal pig section, and evaluate the performance of our methods by the quality of the mapping between the spatial segmentation and the morphological and functional structures (Figure 2). We show that statistical regularization improves accuracy and interpretation of the spatial segmentation over existing approaches.

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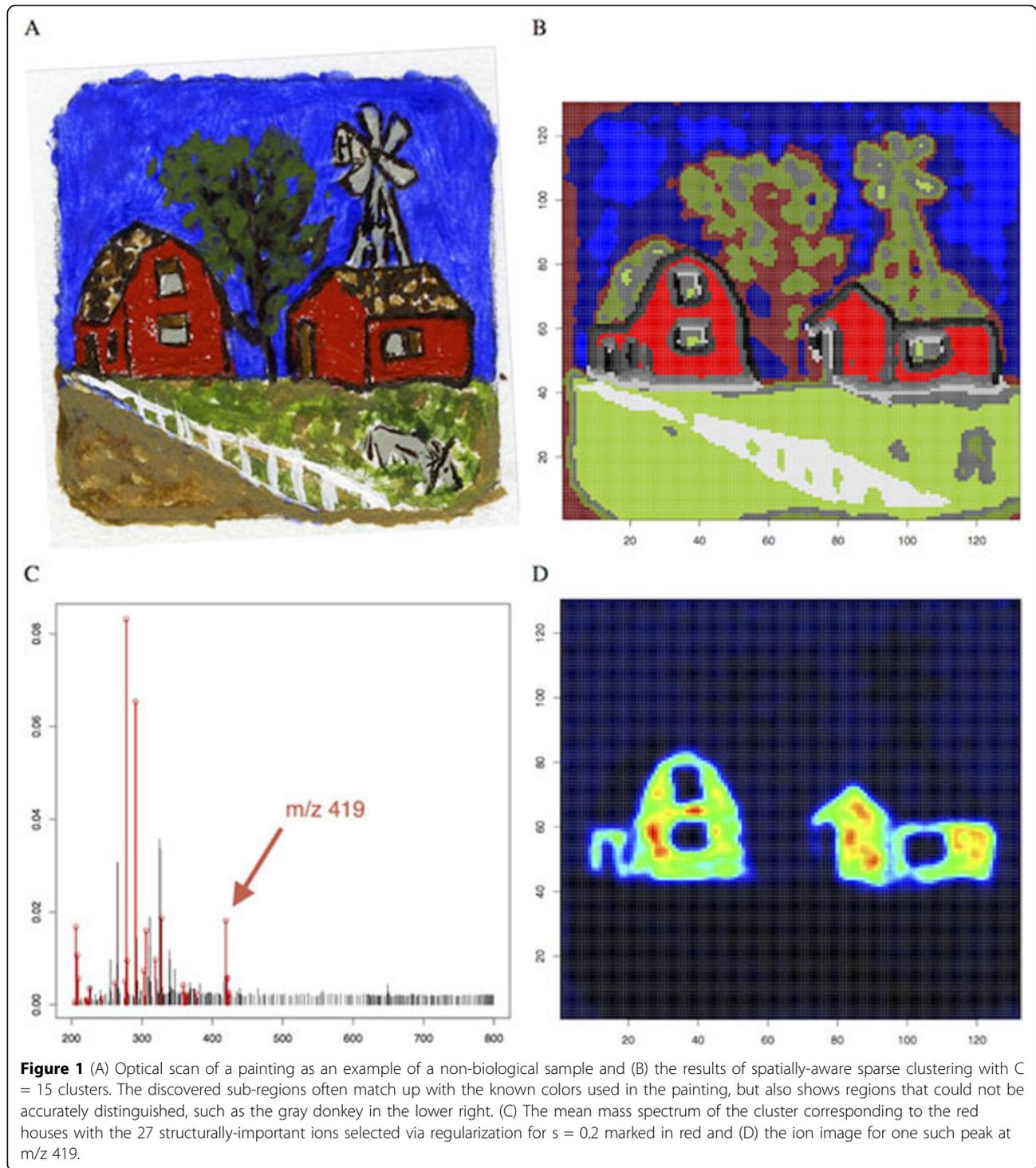
Reference

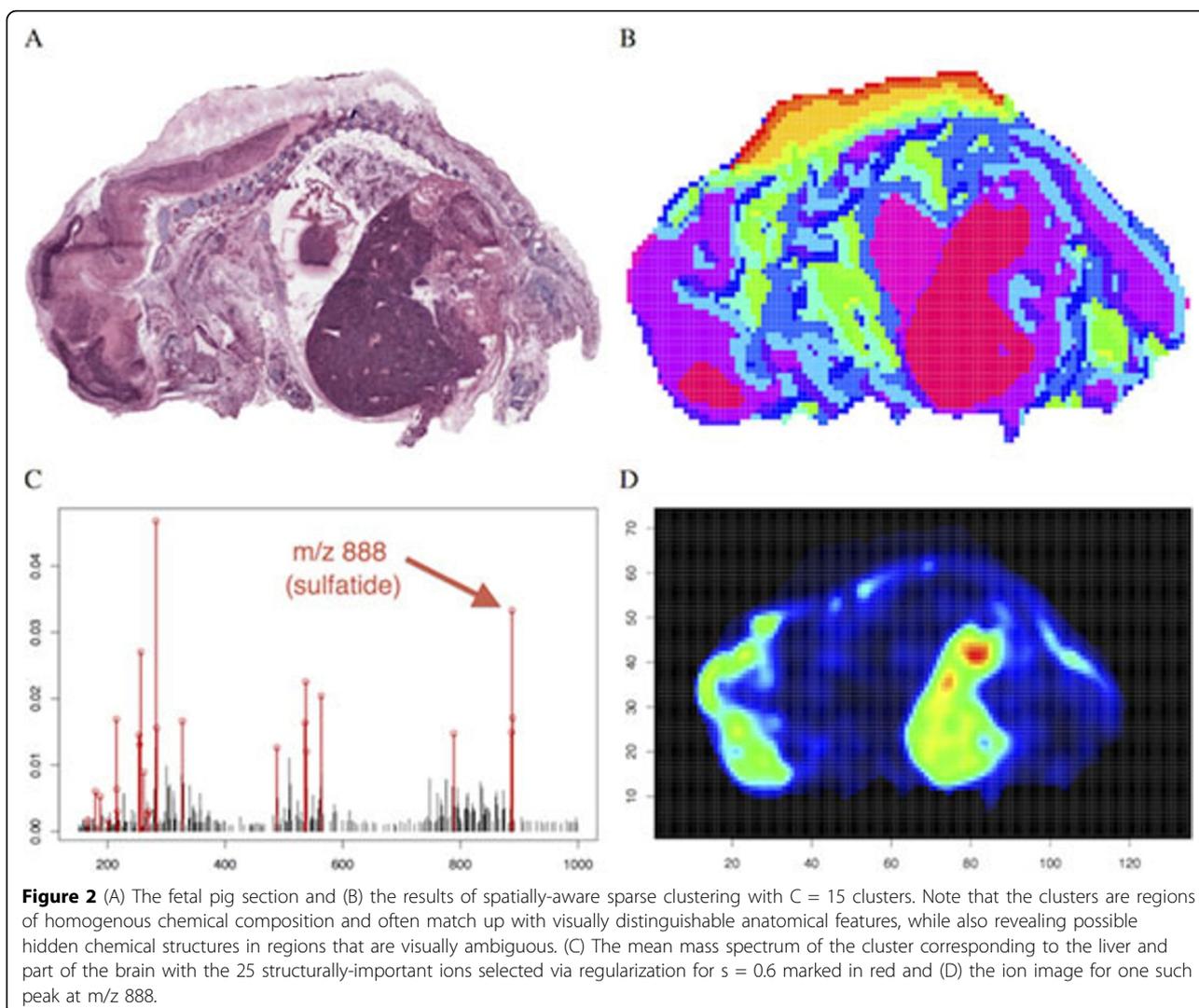
1. Alexandrov T, Kobarg JH: Efficient spatial segmentation of large imaging mass spectrometry datasets with spatially aware clustering. *Bioinformatics* 2012, **27**(13):i230-238.

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