CLUSTERING METHODS IN MA-XRF DATA ANALYSIS

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Introduction

X-ray fluorescence (XRF) spectrometry has been proven to be a core, non-destructive, analytical technique in cultural heritage studies, mainly because of its non-invasive character and ability to reveal the elemental composition of the analyzed artifacts rapidly. With the recent advances in scanning XRF spectrometers capable of attaining data on macroscopic dimensions (MA-XRF), XRF is excessively used for the in situ analysis of works of art. As spectral data are high dimensional, intelligent data analysis methods are needed to achieve data summarization and visualization to conclude the existence of patterns and structures. Cluster analysis in X-ray fluorescence data processing is a constantly evolving field. For this reason, in recent years, several clustering methods have been proposed [1-2], each of which yields interesting results. On the one hand, the diversity of approaches and methodologies equips us with many tools to analyze the vast and diverse amount of data resulting from X-ray fluorescence. On the other hand, the profusion of options confuses. In this work, we survey two data analysis methodologies aiming to study an 18th-century Greek religious icon (i.e., panel painting) to a small number of distinct clusters that involve comparable spectra.

Data acquisition

In our experiment, spectra were collected with a MA-XRF scanner (M6 Jetstream, Bruker), as shown in Figure 1. The M6 Jetstream has a 30 W Rh X-ray tube with polycapillary optics. The present measurements were performed with a high voltage of 50 kV and a current of 600 μA. We scanned a part (242X291 pixels) of an 18th-century Greek religious icon (i.e., panel painting) with a beam spot of 580 μm. as shown in Figure 1&2.

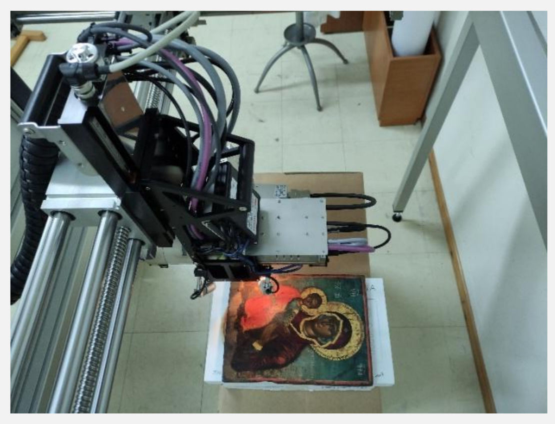


Figure 1: M6 Jetstream (Bruker) MA-XRF Scanner.

Figure 2: Virgin Mary "Odigitria".

Methodology

Our approach for MA-XRF data interpretation is based firstly on applying the k-means clustering algorithms to group the spectra with common features. This procedure groups the ~70K spectra in the X-ray cube spectrum into ten distinct clusters. Then, principal component analysis (PCA) and t-distributed stochastic neighbor embedding (t-SNE) statistical methods are applied to the X-ray cube spectrum to allow for the visualization of the high-dimensional data. Then, we use the log-log square root transformation of the original spectrum to achieve some normalization.

Results

In Figure 3, we show the spatial distribution in two, and three-dimensional scatter plots after k-means application in our data and dimensionality reduction algorithm. In Figure 4, we show the results of the method after the log-log square root normalization.

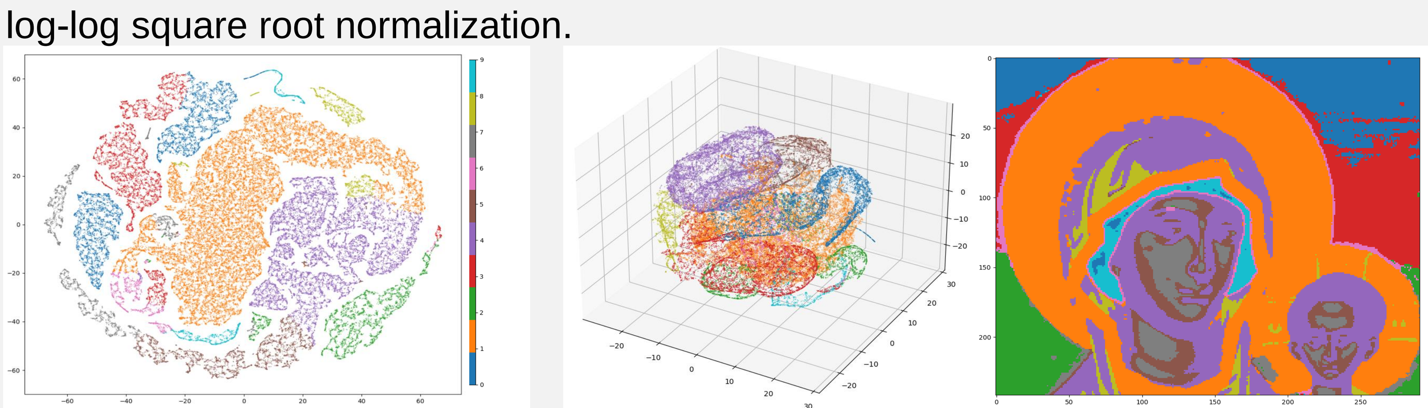


Figure 3: Linear normalization. **Left)** Two-dimensional scatter plot of ten clusters, **Center)** Three-dimensional scatter plot of ten clusters, **Right)** Clusters distribution in the real space of the icon.

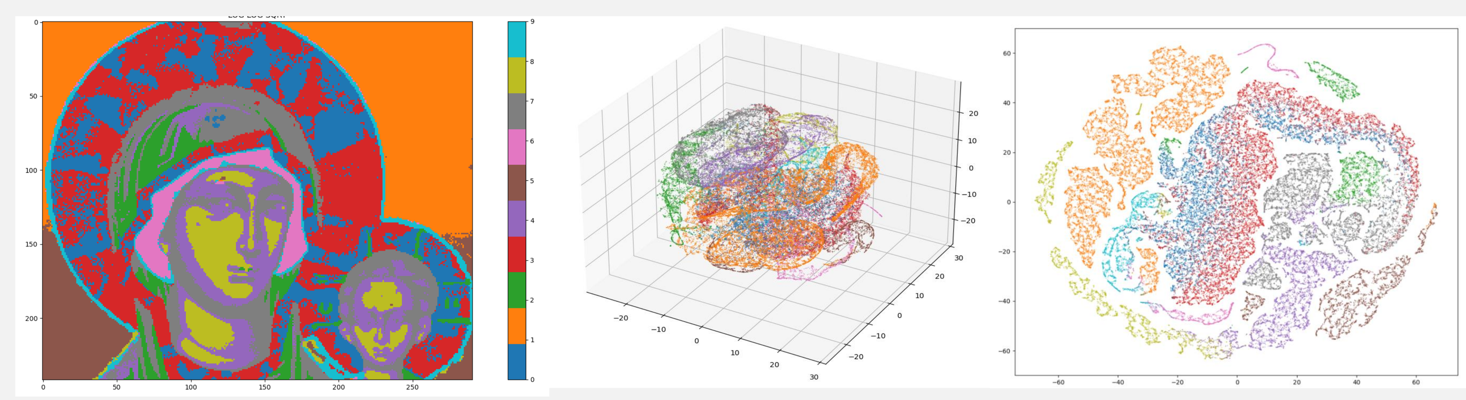
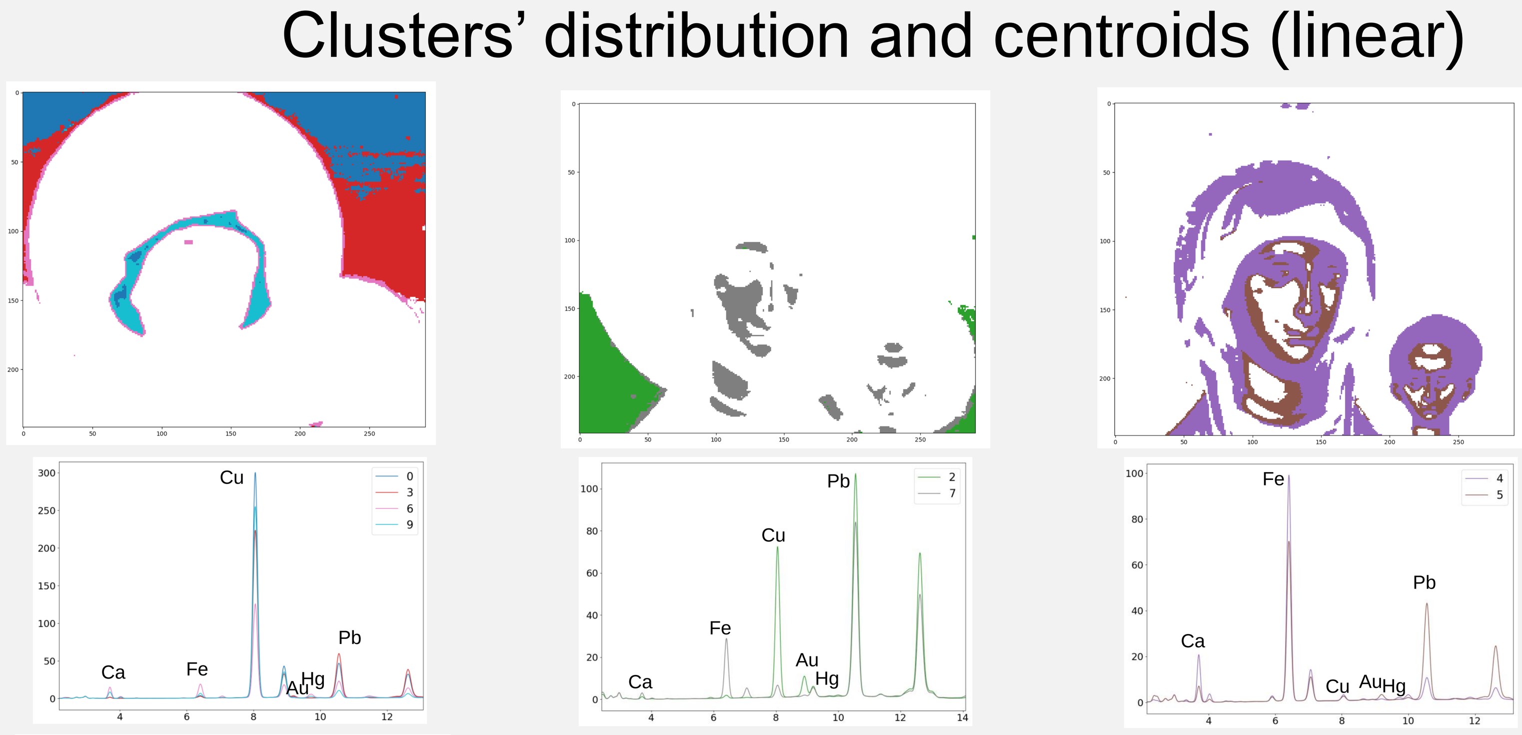
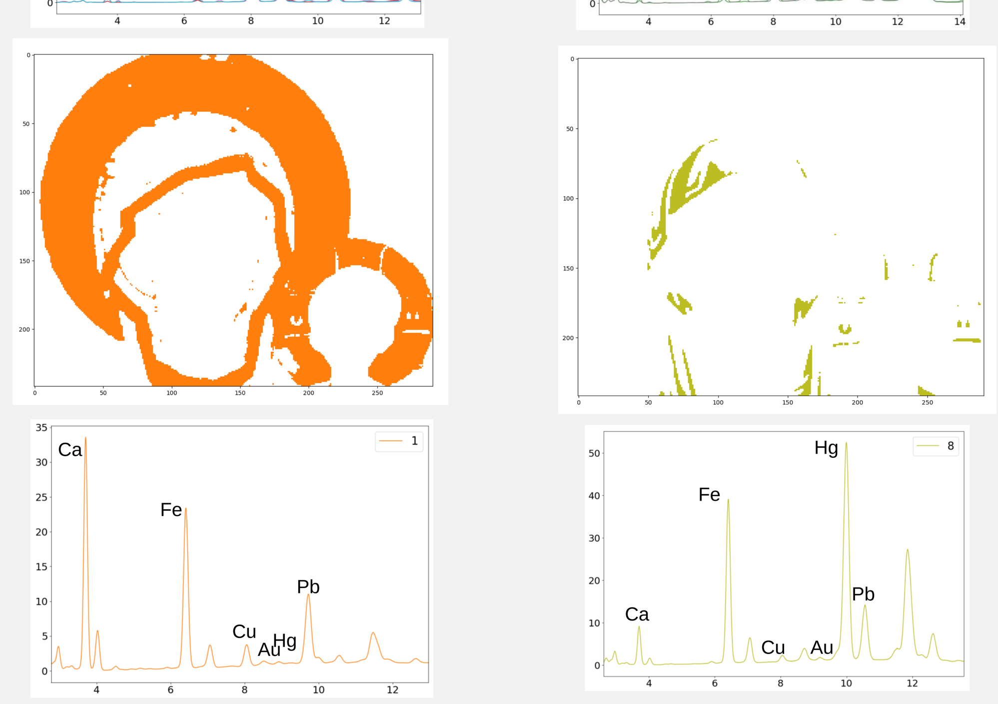


Figure 4: log-log root square normalization. **Left)** Clusters distribution in the real space of the icon, **Center)** Three-dimensional scatter plot of ten clusters after normalization. **Rght)** Two-dimensional scatter plot of ten clusters after normalization.

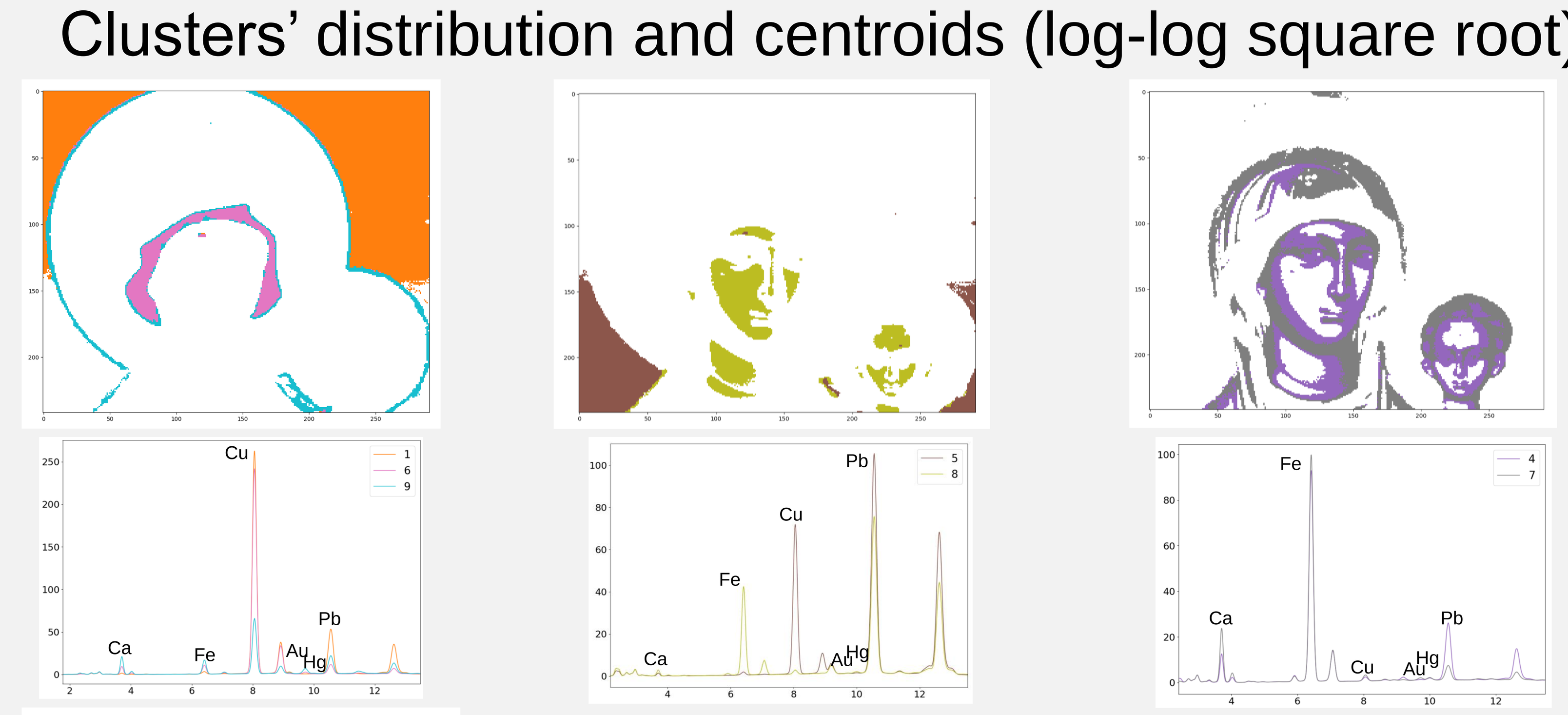
Clusters' distribution and centroids (linear)

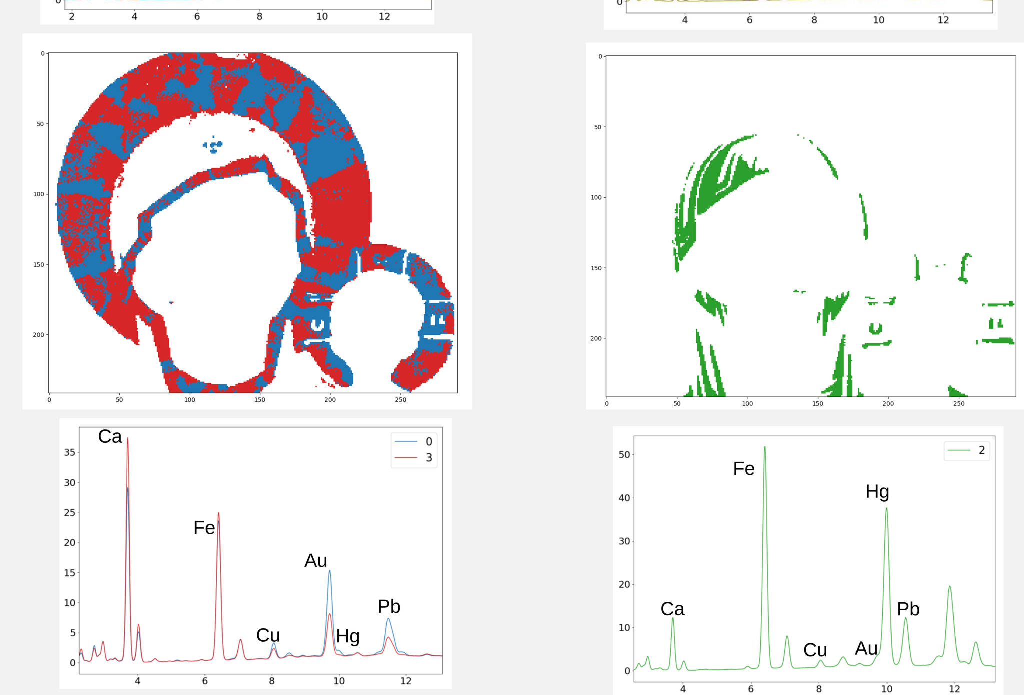




In this case, Cu Kα transition dominates in four clusters (0, 3, 6, and 9). In Virgins Mary's mantle, the cluster distribution perfectly matches the corresponding elemental map. It is also evident that the entire halo becomes a unique Ca dominated cluster (1). However, it contains gold, as shown in the painting and the Au elemental map (Figure 5).

Clusters' distribution and centroids (log-log square root)





In this case, low-intensity elements acquire sufficient weight to form clusters due to normalizing the intensities with the log-log square root. Despite the fact that Cu dominated clusters lose resolution, we observe a Au dominated cluster (0) and a separate Ca dominated that corresponds perfectly with elemental maps. Also Hg cluster (2) fits better with the correspondence elemental map (Figure 5).

Figure 5: Elemental maps distribution.

Conclusions

This work compares two clustering approaches in X-ray fluorescence data analysis. We study dimensionality reduction algorithms and show a way to emphasize elements with lower intensities with a previous normalization of the data set. As a result, the cluster analysis gives different results. Finally, from the two approaches, it becomes clear that no unique approach can work optimally in all cases.

References

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Acknowledgments

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