MA-XRF and machine learning techniques for image digital restoration and elemental maps prediction

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Scanning X-ray fluorescence spectrometry (MA-XRF) allows the non-destructive analysis and characterization of painted objects, whose visual appearance is strongly correlated to the used painting materials and techniques. The application of MA-XRF in the study of paintings permits the extraction of elemental distribution maps. This work firstly presents the correlation of MA-XRF spectra with the visual RGB colors of a religious panel painting ("icon") by applying advanced computational machine learning techniques, like regression and deep learning neural networks, in order to associate the color rendering with the spectral information. It is thus demonstrated that through this methodological approach, hidden or faded appearance of the artifact can be unveiled. On the other hand, with advanced machine learning techniques, elemental mapping of the main elements of paintings can be predicted. The potentials of the applied methodology are showcased on an 18th-century Greek icon of Virgin Mary "Odigitria".

RGB correlation with regression and autoencoders

figure 1

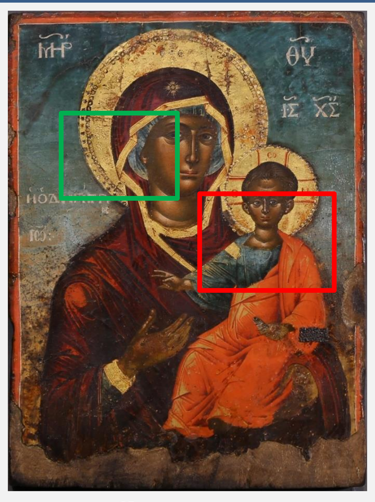
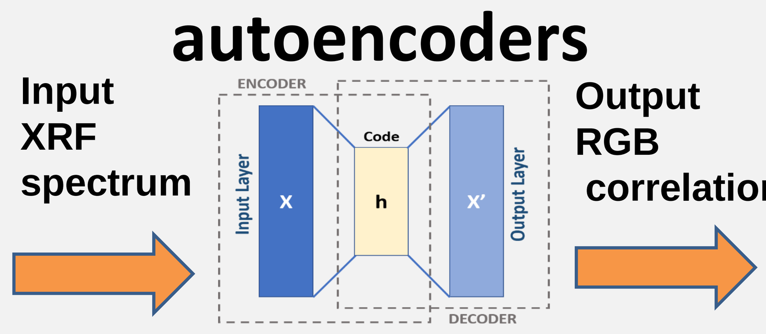


figure 2



In the first experiment we have scanned two areas, one at the Virgin Mary's face and a second at Jesus' face and clothes as shown in figure 2. XRF scanning was performed using the M1-Mistral Bruker (figure 1) micro-XRF spectrometer which is equipped with a thick glass window (of ~2 mm thickness) microfocus X-ray W-tube, providing a continuous excitation spectrum emerging from 10 keV. Interchangeable beam collimators determine the beam spot on the target. The sample is positioned on a motorized X-Y-Z translation table. We scanned the selected areas as shown in figure 2. The beam spot was 1 mm for Virgin Mary's face (green frame, 2665 spectra) and 2 mm for Jesus' face (red frame, 1426 spectra). Then we use the first data set and its RGB correlation as training set for a machine learning algorithm in order to learn the RGB correlation of each spectrum and after that we checked the efficiency of the algorithm with the red one (Jesus' face).

Firstly we experimented with regression algorithms like lasso, knn and svm regression. The best score accumulated knn regression with 10 nearest neighbors and eukledean metric (score 0.45). The result is shown in figure 3.

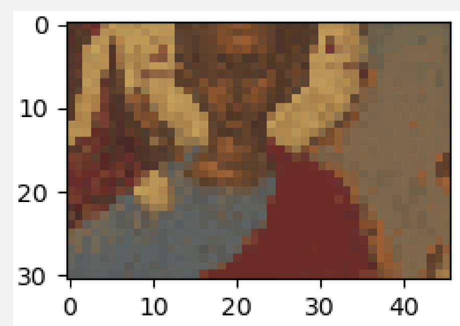


figure 3

figure 4

Secondly we tried to train an autoencoder (5 intermediate downsampling and upsampling layers (Linear + ReLU)).

Decoder: L2 Loss (*DecLoss*)

Encoder: *DecLoss* + c·*EncLoss*

Autoencoder is a self-supervised method aiming at leveraging the underlying structure in the data. Initially we trained only an encoder to learn the mapping from spectra to rgb (RGB_target_values). During training, encoder's loss (RGB_Loss) is consecutively backpropagated in order to update its parameters and finally to learn the best mapping. Then, we investigate whether the latent spectral representations produced by the autoencoder enhance the encoder's performance by combining the decoder's backpropagated loss (Reconstruction_Loss) with the RGB_Loss, having defined the number of dimensions in latent space to 3, in correspondence to RGB dimensions. The results are shown in figure 4.

Elemental maps predictions with artificial neural networks

First experiment

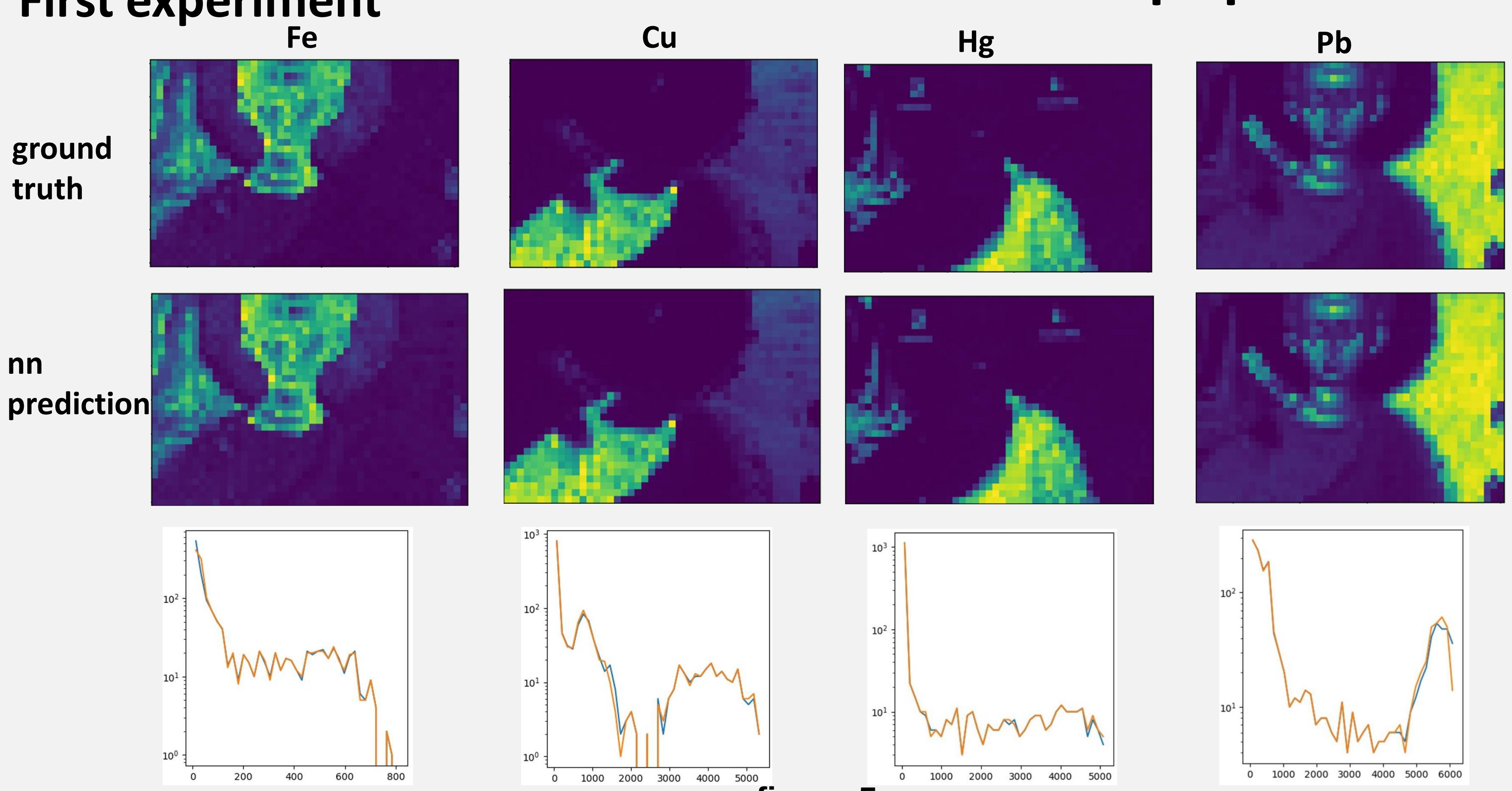
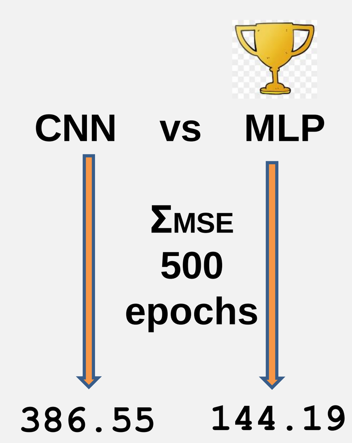
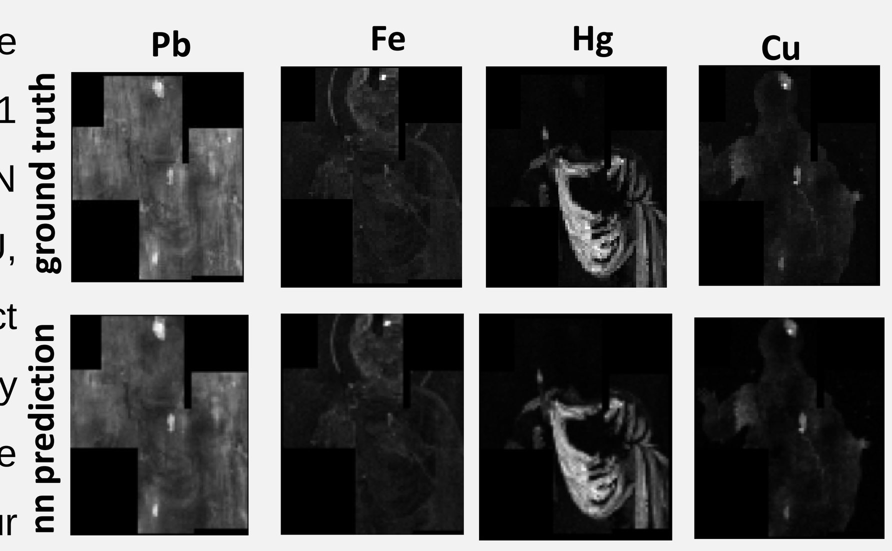


figure 5



Next step was to train with the same dataset an MLP (Multilayer Perceptron) (1 hidden layer, 100 neurons) and a CNN (Convolutional Network) (Conv1d, RELU, MaxPool, Linear) [1,2] in order to predict elemental maps. The spectra were firstly analyzed with PyMCA for extracting the counts per pixel per each element, in our case Ca, Mn, Fe, Cu, Ag, Au, Hg and Pb, as target vector for each spectrum. MLP gave us better results (figure 5) than the CNN. Finally we use another dataset (S. Fanourios, shown in figure 6) that was not used for the training in order to verify the robustness of our method.



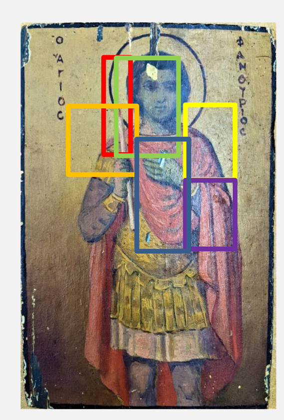


figure 6

- 6 areas scanned
- 1 mm step on both axes
- more than 4500 spectra
- over 13 hours of operating time
- 5 seconds per measurement
- Cu appears on the substrate

Second experiment

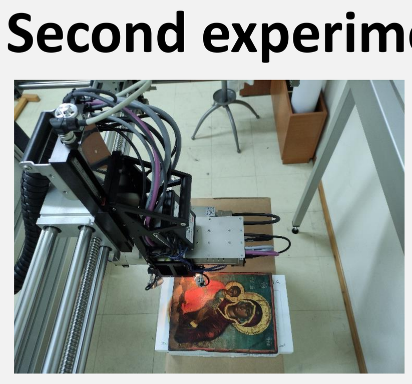


figure 7

In this experiment, spectra were collected with a MA-XRF scanner (M6 Jetstream, Bruker, figure 7). The M6 Jetstream is equipped with a 30 W Rh X-ray tube with polycapillary optics, in our case operated at 50 kV and 600 μA. All spectra (~240 K spectra) were collected with 580 μm beam spot. We train a MLP with a hidden layer for predicting elemental maps of the same 8 elements (figure 8&9). We checked the results in a religious painting panel (St.Ioannis, 274x367 pixels) that was not used for the training. The results are shown in figure 10.

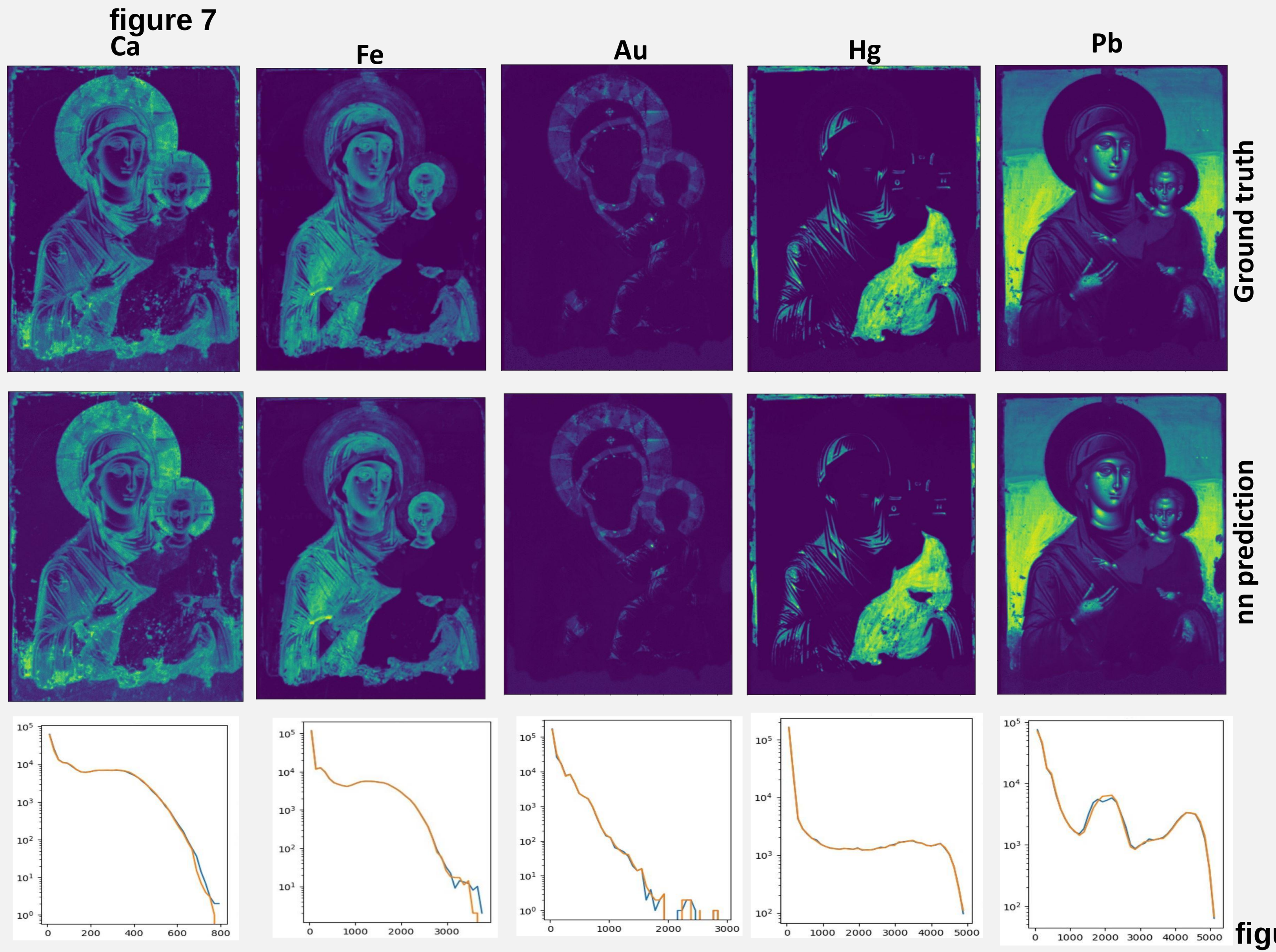
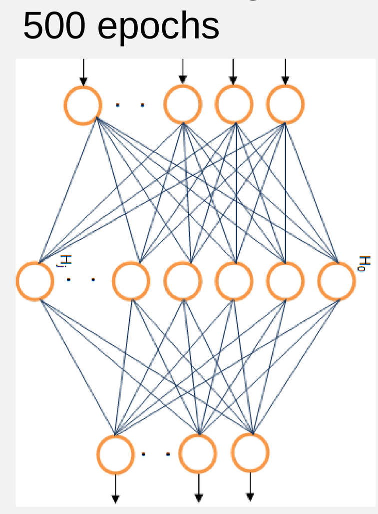


figure 8

input:
4096 channels

Training:
41000 spectra
0.005 learning rate
500 epochs

hidden layer:
200 neurons
RELU



output:
8 elements
Ca, Mn, Fe, Cu,
Ag, Au, Hg, Pb

figure 9

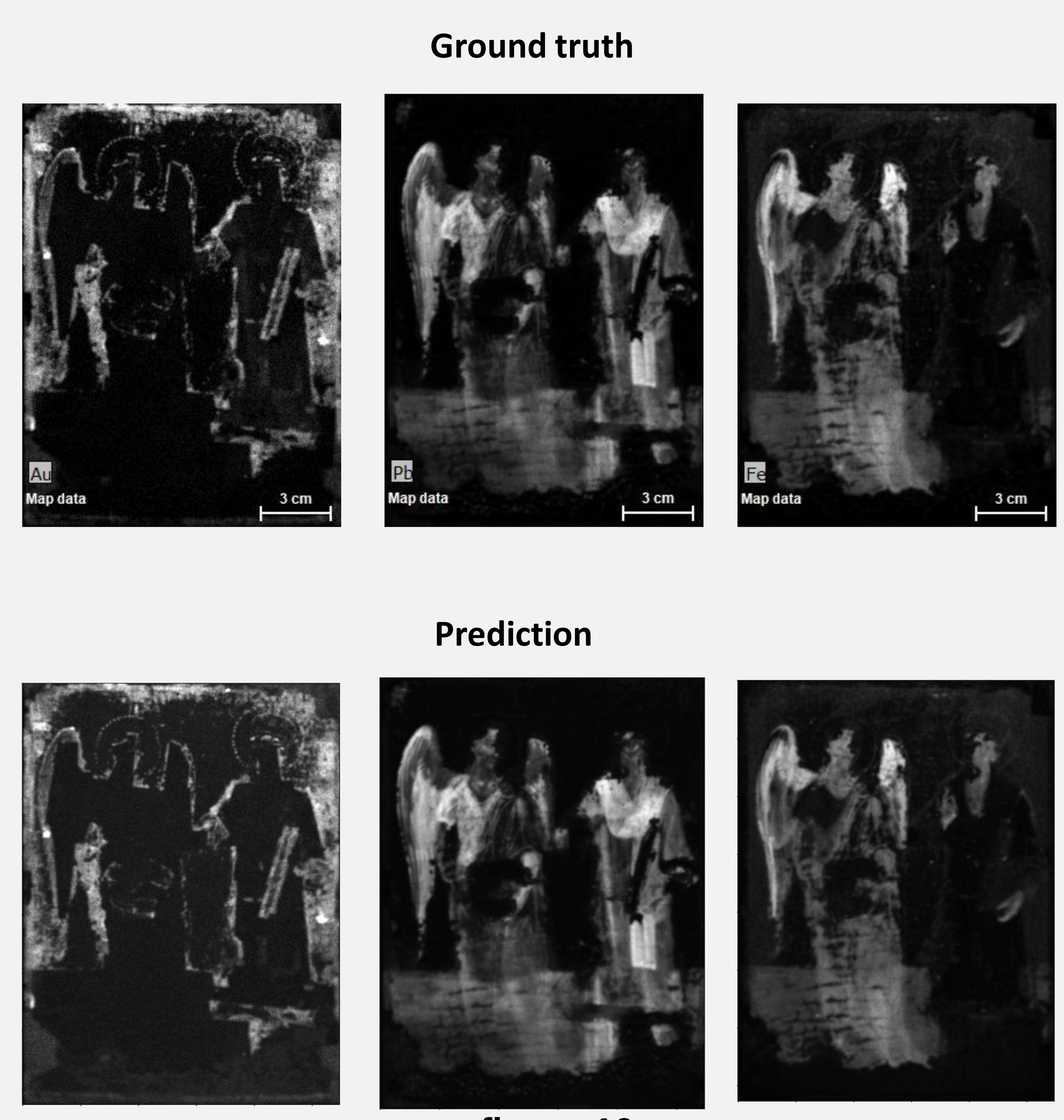


figure 10

Conclusions

In this work we show how with advanced computational machine learning techniques we can associate the color rendering with the spectral information. This methodological approach is very important because hidden or faded appearance of the artifact can be unveiled. Also, we show how elemental mapping intensity analysis of paintings can be predicted with the use of neural networks, fact equally important in the speed of analysis, but also for inexperienced users of MA-XRF. It is worth mentioning that MLP gave better results than CNN to the specific problem.

References

[1] Jones et al. 2022. "Neural Network-Based Classification of X-Ray Fluorescence Spectra of Artists' Pigments: An Approach Leveraging a Synthetic Dataset Created Using the Fundamental Parameters Method." Heritage Science 10 (1): 88. https://doi.org/10.1186/S40494-022-00716-3.

[2] Preisler et al.2022 "Deep Learning Models for MA-XRF Imaging Spectroscopy of Paintings." Conference: Computational approaches for technical imaging in cultural heritage (7th IP4AI meeting), 27–29th April 2022

Acknowledgments

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