RAMAN SPECTROSCOPY DECONVOLUTION USING STACKED AUTO-ENCODERS WITH NON-NEGATIVITY CONSTRAINTS

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ABSTRACT

Index Terms— One, two, three, four, five

1. INTRODUCTION

Surface-enhanced Raman scattering (SERS)

Hotspots, complex mixture in raman spectra.

NMF/MCR for source seperation and mixture classification.

Computational heavy for increased resolution of Raman spectras.

Sparse autoencoder

2. PRIOR WORK

Primary reference [1]

3. METHODS

Dataset origin, description of wavenumbers, raman map size. Definitions for the rest of the paper.

Compare with NMF?

Add how NMF/MCR is used in raman spectroscopy.

3.1. Non-negative matrix factorization

Non-negative matrix factorization (NMF) consists of factorizing a original matrix V, with only positive elements, into two positive matrices W and H. [2]

$$V \approx W \times H \tag{1}$$

Where columns of W are considered basis vectors, and each column in H is considered an encoding with a one-to-one relationship with the columns of V. So for instance, a matrix V of size $n \times m$ can be factorized into a matrix W of size $n \times k$ and a matrix H of size $k \times m$, where k is the number of components. Completing the intuitive point of view, W and W can be seen as components that combined approximate the original signal V.

Thanks to XYZ agency for funding.

An iterative algorithm is considered for NMF, which shares similar monotonic convergence as the EM algorithm. [3]. Moreover, the rules of update preserve non-negativity of W and H. The algorithm approaches the problem by initialization of W and H as non-negative, and then update the values in W and H until local maximima is obtained and the both matrixes are considered stable. The rules of multiplicative update can be defined as:

$$H^{n+1} \leftarrow H^n \frac{(W^n)^T V}{(W^n)^T W^n H^n} \tag{2}$$

and

$$W^{n+1} \leftarrow W^n \frac{V(H^{n+1})^T}{W H^{n+1} (H^{n+1})^T} \tag{3}$$

3.2. Sparse auto-encoder with non-negativity constraint

Reconstruction of input vector through unsupervised learning. Parametric deterministic mapping [4]

$$y = f(x) = \mathbf{W}x + \mathbf{b} \tag{4}$$

Where x is the input vector and $\mathbf{W}$ is a mtrix of weights and $\mathbf{b}$ is a bias vector. y is the latent representation that is reconstructed in input space by

$$z = g(y) = \mathbf{W}'x + \mathbf{b}' \tag{5}$$

Primary reference implementation. Describe the constraint and the training architecture

3.3. Latent-space classification

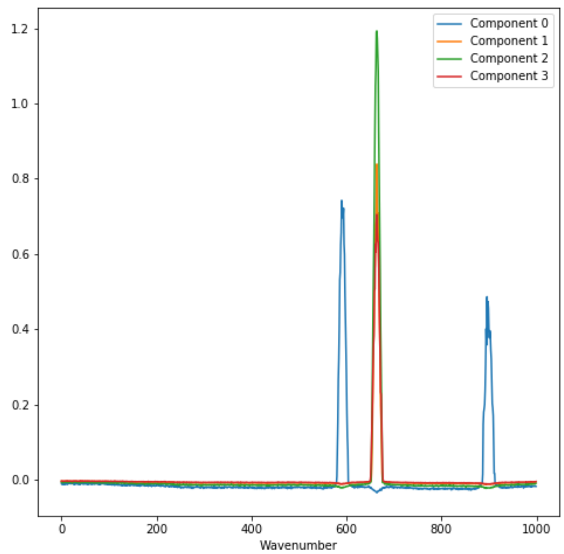
classification based on latent-space by compression of sparse autoencoders.

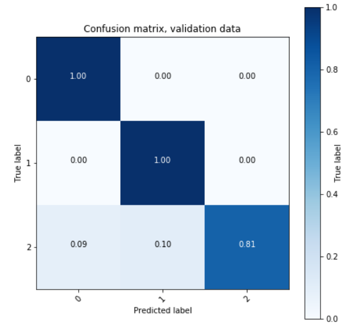
4. RESULTS

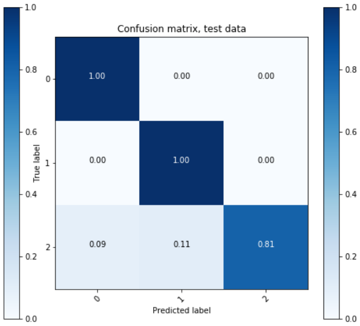
Training and test data.

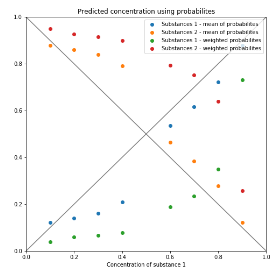
Encodings and basis vectors

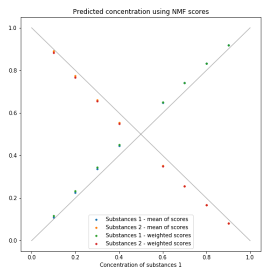
Classifier results

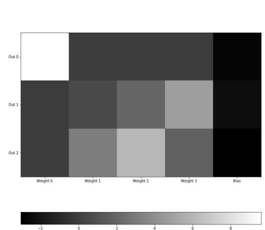


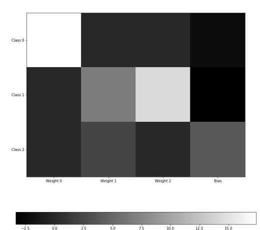


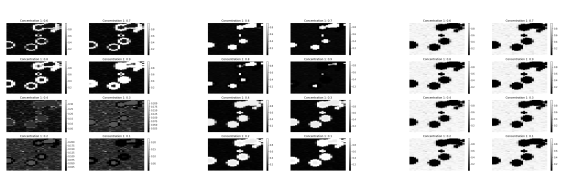


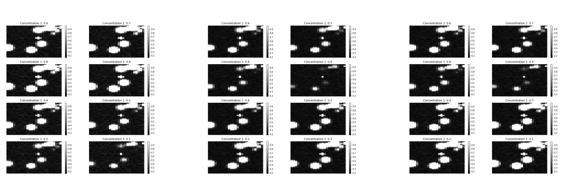












5. DISCUSSION

Comparison with NMF

6. CONCLUSION

7. REFERENCES

List and number all bibliographical references at the end of the paper. The references can be numbered in alphabetic order or in order of appearance in the document. When referring to them in the text, type the corresponding reference number in square brackets as shown at the end of this sentence .

8. REFERENCES

[1] Ehsan Hosseini-Asl, Jacek M. Zurada, and Olfa Nasraoui, "Deep Learning of Part-Based Representation of Data Using Sparse Autoencoders With Nonnegativity Constraints," *IEEE Transactions on Neural Networks and Learning Systems*, vol. 27, no. 12, pp. 2486–2498, dec 2016.

[2] H. Sebastian Seung and Daniel D. Lee, "Learning the parts of objects by non-negative matrix factorization," *Nature*, vol. 401, no. 6755, pp. 788–791, oct 1999.

[3] A. P. Dempster, N. M. Laird, and D. B. Rubin, "Maximum Likelihood from Incomplete Data via the EM Algorithm," 1977.

[4] Pascal Vincent, Hugo Larochelle, Yoshua Bengio, and Pierre-Antoine Manzagol, "Extracting and Composing Robust Features with Denoising Autoencoders," .