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Hyperspectral unmixing for Raman spectroscopy via physics-constrained autoencoders

Raman spectroscopy is widely used across scientific domains to characterize the chemical composition of samples in a nondestructive, label-free manner. Many applications entail the unmixing of signals from mixtures of molecular species to identify the individual components present and their proportions, yet conventional methods for chemometrics often struggle with complex mixture scenarios encountered in practice. Here, we develop hyperspectral unmixing algorithms based on autoencoder neural networks, and we systematically validate them using both synthetic and experimental benchmark datasets created in-house. Our results demonstrate that unmixing autoencoders provide improved accuracy, robustness, and efficiency compared to standard unmixing methods. We also showcase the applicability of autoencoders to complex biological settings by showing improved biochemical characterization of volumetric Raman imaging data from a monocytic THP-1 cell (Figure 1).

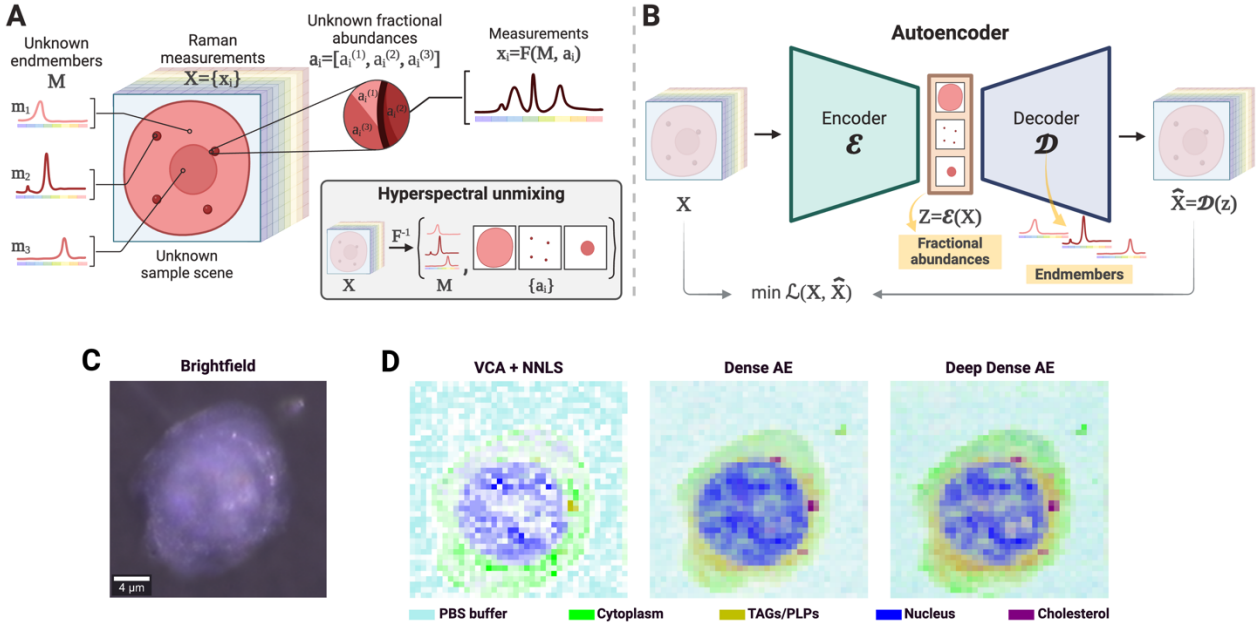

Figure 1: Improved Raman cell imaging via Raman unmixing autoencoders. (A) Illustration of cell imaging via hyperspectral unmixing. (B) Hyperspectral unmixing as a self-supervised autoencoder learning problem. (C) Brightfield image of the studied THP-1 cell (data from Kallepitis et al. (2017) [1]). (D) Image reconstructions of the cell obtained by: a standard method for unmixing - VCA [2] + NNLS [3]; our dense autoencoder model; and a deeper version of our dense autoencoder.

References

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[3] C. L. Lawson, R. J. Hanson, Solving Least Squares Problems (SIAM, 1995).