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Comparison Between Deep Learning and Iterative Bayesian Statistics Deconvolution Methods in Energy Electron Loss Spectroscopy

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In recent years, the application of Artificial Intelligence (AI)-driven methods for improving data analysis in multiple scientific fields has drastically increased. Therefore, thoroughly evaluating the performance of such new methods is of great importance, in particular in comparison with other commonly used techniques. In this study, a recently developed deep learning deconvolution software named EELSpecNet [1] is evaluated and compared with a commonly used iterative Bayesian method known as the Richardson-Lucy (RL) algorithm applied in the field of Electron Energy Loss Spectroscopy (EELS) [2]. In order to compare the performance of iterative and deep learning approaches, both techniques are used for low-loss EELS signal reconstruction (deconvolution) including the contribution and extraction of the zero-loss peak signal. A set of randomly generated spectra, including common experimental artifacts such as electron beam energy jitters, optical transfer function convolution (broadening), and high-frequency electronic noise is first used to train the EELSpecNet network. Another similar set of spectra was then utilized to evaluate the technique and compare different aspects of signal restoration using these different methods.

According to quantitative analysis carried out for both techniques, by increasing the high-frequency noise amplitude in the distorted spectra, the RL method not only does show noise reduction properties but can drastically increase the variance of high-frequency noise in the deconvolved signal by a factor of 4. In contrast, our results show that, taking advantage of its U-shaped deep neural network architecture, EELSpecNet data processing demonstrates a robust noise cancelling feature, reducing the noise variance by a factor of 40, while not being considerably affected by the noise amplitude in the distorted data. Figure 1 shows an example of EELSpecNet performance in restoring original reality of a noisy spectrum. The deep learning method’s capability to remove background signals, normally a serious issue in low-loss EELS data extraction, especially near the zero-loss peak, is also compared with the RL iterative technique. In this context, our results show that the deep learning solution outperforms RL in background removal. In this regard, the relative error distance in the full width at half maximum (FWHM) and full width at tenth maximum (FWTM) of the reconstructed signal for EELSpecNet is 0.03% and 0.002% respectively while, in comparison with the same data after 50 iterations of RL, the relative error distance is around 300% and 400% respectively; see Figure 2. The fidelity of the deconvolved signal with the original signal is measured using the structural similarity index suggested by Z.Wang [3, 4], which clearly demonstrates that a deep learning solution is better than the utilized Bayesian algorithm.

In conclusion, the current study investigation demonstrates that the deep learning method outperforms the widely used RL algorithm when the network is properly trained. Nevertheless, the comparison cannot be extrapolated to the aspects and features that were not considered in the training data. In this regard, although EELSpecNet shows great advantages in this specific domain, its application in a more general scheme would require the model to be trained on the relevant experimental conditions [5].

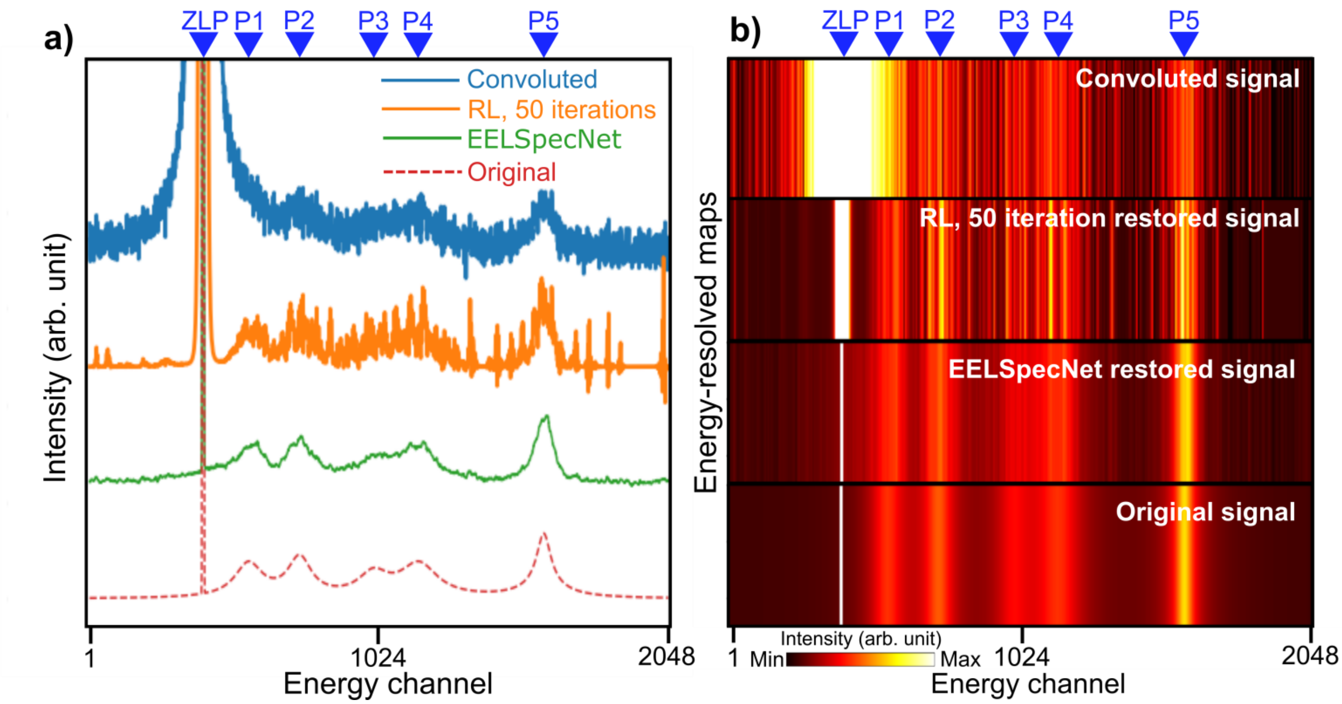

Figure 1. a) An example of a distorted low-loss EELS spectrum (blue curve), deconvolved using 50 iterations of RL (orange curve), and EELSpecNet (green curve). The original spectrum is shown using a dashed red curve. b) To better compare the restoration power of the deconvolution methods and similarity of the deconvolved spectra, their energy-resolved maps of spectra in (a) are depicted.

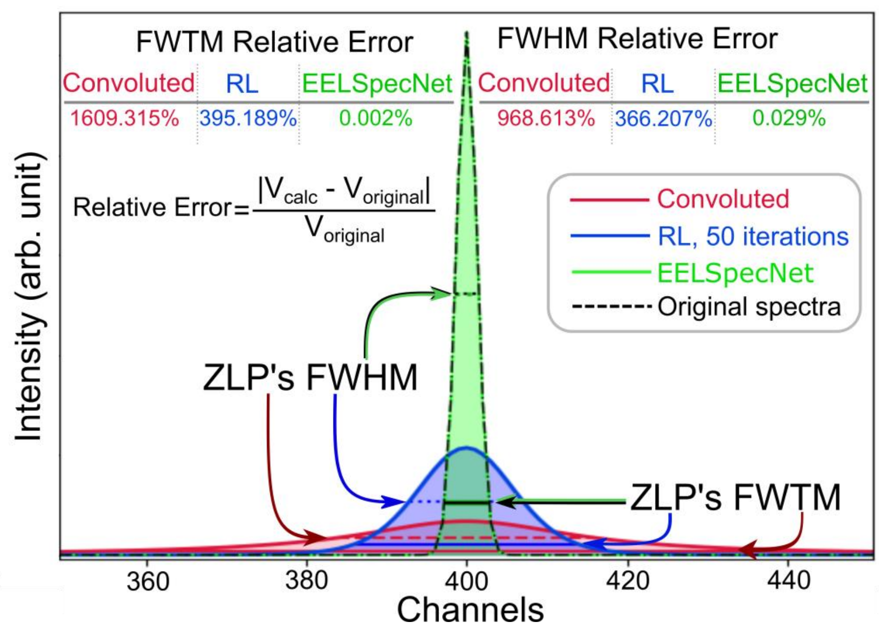

Figure 2. Magnified near the zero-loss peak (ZLP) region of the original, convoluted, and deconvolved version of an EELS spectrum. Relative error in full width at half maximum (FWHM), and full width at tenth maximum (FWTM) of the ZLP before and after deconvolution demonstrates advantage of EELSpecNet in restoring the near-ZLP region. The red curve represents convoluted signal, the blue curve is the deconvolved signal after 50 iterations of the RL algorithm, the green curve is the restored signal using EELSpecNet, and the black dashed curve is the original signal.

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