

Bridging Spectroscopic Data-Driven Modeling to Clinical Applications

Oleg Ryabchykov, Leibniz Institute of Photonic Technology, Leibniz Institute of Photonic Technology, Member of Leibniz Health Technologies, Member of the Leibniz Centre for Photonics in Infection Research (LPI), Jena, Germany

Abstract

Recent advances in data-driven modeling for spectroscopic and imaging modalities have significantly expanded the capabilities of optical diagnostics. One of the factors behind this progress is the growing integration of data-driven strategies throughout the spectroscopic workflow. Deep-learning architectures originally developed for imaging, such as U-Net variants, are now widely adapted to Raman and infrared spectra, where they effectively suppress noise while preserving diagnostically relevant features.¹ This improves spectral data quality and consistency across varied acquisition conditions.

As modeling strategies become more sophisticated, interpreting their behavior remains challenging. Explainable AI techniques offer partial insight, yet models that appear interpretable may still produce overly confident errors. Evaluating model uncertainty through approaches such as Monte Carlo dropout provides a way to identify unreliable predictions and filter ambiguous spectra during training, which can lead to more robust test performance.²

Developments in data-driven methods can substantially strengthen the reliability of vibrational spectroscopy. At the same time, they underscore the need for further progress in standardization, uncertainty handling, and model transparency. Continued work in these areas will be essential to ensure that spectroscopic modeling becomes robust enough for routine clinical use.

References

¹ Mokari, A., et al. "A comparative study of robustness to noise and interpretability in U-Net-based denoising of Raman spectra." *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (2025): 126577.

² Contreras, J., et al. "ATR-FTIR Spectroscopy of Saliva and Machine Learning as a Screening Test for Sjögren Disease." *Analytical Chemistry* 97.47 (2025): 26034-26044.