Contribution ID: **26** Type: **not specified**

Empowering Spectroscopic Technologies: Streamlining Calibration Model Development and Online Monitoring with Bayesian Optimization

Thursday, 29 May 2025 15:35 (3 minutes)

Spectroscopic technologies have seen a substantial rise in applications in recent years, particularly in the monitoring of cell cultures. In addition to this established use, novel applications are emerging, such as the utilization of spectroscopic techniques in microbial fermentations. Alongside these advancements, innovative methods are being developed to create calibration models that effectively correlate spectral measurements with reference concentrations of specific species. Despite these promising developments, the adoption of spectral technologies, especially among smaller companies, remains limited. This is primarily due to challenges associated with data management, as well as the need for specialized knowledge in data analytics and modeling, which can pose a barrier for non-experts.

In this contribution, we present a streamlined approach to calibration model development by employing Bayesian optimization for hyperparameter tuning. This advanced technique enables the automatic selection of data treatment methods, preprocessing techniques, and modeling algorithms, significantly reducing the effort required to develop robust and reliable calibration models. By automating key and complicated aspects of the process, Bayesian optimization empowers users who may lack specialized data analysis skills, thus lowering the entry barrier for adopting spectroscopic methods.

Furthermore, we demonstrate the advantages of implementing this approach on a cloud-based platform, where data is consistently contextualized and made accessible to various stakeholders. Such a platform fosters collaboration among individuals with diverse expertise, promoting more integrated and efficient model development workflows.

Our findings emphasize the potential of Bayesian optimization as a powerful tool for simplifying and democratizing the use of spectroscopic technologies. By enabling more efficient calibration model development and supporting online monitoring, this approach can significantly accelerate the adoption of spectroscopic methods in both research and industrial settings.

Type of presentation

Poster

Primary author: RESSURREIÇÃO, Miguel (DataHow AG)

Presenter: RESSURREIÇÃO, Miguel (DataHow AG)

Session Classification: Poster

Track Classification: Spring Meeting