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**How 'Explainable ML' Can Improve Process Performance**

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ABSTRACT

This study introduces a novel framework that leverages explainable machine learning for image analysis to predict and analyze process performance in biomanufacturing. Our approach transforms process sensor data into spectrograms, which are then used to fine-tune a pre-trained convolutional neural network for accurate performance prediction. To enhance transparency, we apply Grad-CAM, an interpretability technique that highlights key signals, filters out non-critical factors, and pinpoints the most influential time periods during the process.

We demonstrate our method through a case study addressing a reduction in binding capacity during column chromatography, using wash and equilibration data. Remarkably, the model achieved reliable predictions with a modest training dataset of only 130 examples. As expected, UV absorbance proved to be the most influential parameter, while conductivity and pressure played a lesser role. Notably, the model also identified the change in UV absorbance before and after elution—an effect attributed to the gradual oxidation of DTT in the buffer system.

Our findings suggest that this framework has broad applicability for analyzing complex chemical and bio processes with limited data, enabling the identification of critical process parameters and time windows that might otherwise be overlooked by conventional methods. This allow to fine tune chemical process to improve overall process performance.

KEY WORDS

AI, Bioprocessing, Process prediction

BIOGRAPHY

Lukas Gerstweiler is a lecturer in Chemical Engineering at the University of Adelaide, where he leads the Biomanufacturing Research Group. His work focuses on continuous biomanufacturing, mRNA and virus-like particle production, and chromatographic purification methods. His research aims to streamline industrial bioprocessing while enhancing product quality.

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