Selective High-Precision Control of Process Variables in Automated Experimentation

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In recent years, the automation of experiments has rapidly advanced in materials science, demonstrating the effectiveness of combining automated systems with machine learning for materials design and reaction condition screening. Automation improves process reproducibility and reduces variability in measured properties through consistent operations.However, high implementation costs often limit its adoption to select institutions or companies. One major factor is the uniform application of high-precision control across all experimental steps, despite the varying requirements for control accuracy depending on the specific variable. These differences are typically addressed implicitly through expert knowledge, lacking quantitative or systematic guidelines.

In this study, we propose a data-driven framework to identify critical experimental variables that require precise control, enabling realistic and efficient optimization using a low-cost automated system.

We constructed an automated setup using the affordable robotic arm “Dobot Magician”, a spray coater, and a hot plate. Experimental data are automatically logged in the electronic lab notebook “eLabFTW”, facilitating seamless integration with Bayesian optimization. Our target is the automated synthesis of TiO_2 photocatalysts via spray pyrolysis. Using photocurrent before and after illumination as the objective variable, we apply Bayesian optimization with Heteroscedastic Gaussian Process Regression to account for experimental uncertainty and to propose variable-specific precision control strategies.