Bayesian optimization for self-driving liquid coating laboratory

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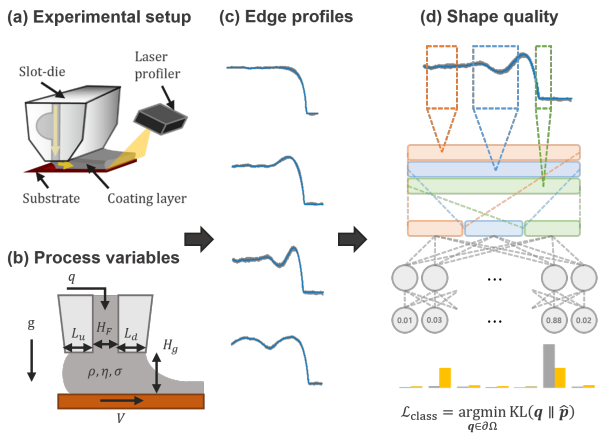

Fig. 1: Schematic diagram of the proposed method for quantifying edge shape qualities.

1. Introduction

Liquid coating is a common process in manufacturing industries, including the fabrication of batteries, displays, semiconductors, solar cells, and many others. Because uniformity of the coated layer is critical to performance of the final product, discovering optimal process conditions to control the surface profile is a key step in process development. In this work, we present a Bayesian optimization framework for controlling the shape of edge profiles in liquid coating processes. The proposed framework can be integrated with a self-driving laboratory platform to enable autonomous optimization of industrial coating processes.

2. Backgrounds

Previously, coating research mainly focused on controlling the global thickness and roughness of the coating layer, and achieving a steady coating condition. However, as coating technologies have advanced, local shape defects that can take place even under steady coating conditions have become more prominent. One such defect is the 'heavy edge' phenomenon, where the edges of the coated layer become thicker than the center region. This phenomenon, which is especially prominent in lithium-ion battery (LIB) electrode manufacturing, can lead to material waste, reduced performance, and even mechanical failures in the final product.

One of the challenges in optimizing edge shapes is the lack of quantitative metrics to evaluate the quality of arbitrary edge shapes. Previous studies have proposed several metrics to quantify local edge shape qualities, but these metrics are limited to specific edge shape types and cannot be generalized to arbitrary shapes. Another challenge is the high cost and time required for experimental trials in coating processes, which makes traditional optimization methods impractical. This issue is further exacerbated by the increasing dimensionality of parameter space in modern coating processes.

To address these challenges, we propose a data-driven framework that leverages feature learning techniques and surrogate modeling to control arbitrary edge shapes in liquid coating processes. The loss function we define successfully represents both the global and local edge shape qualities. By integrating this loss function with Bayesian optimization, we can efficiently explore the high-dimensional parameter space and identify optimal process conditions.

2.1 Related work

The 'heavy edge' phenomenon was already reported in film casting and coating processes[1, 2]. Schmitt et al. investigated this phenomenon in slot-die coating of LIB electrodes, and defined metrics to quantify local shape quality of edges[3]. Several subsequent studies adopted these metrics and studied the effects of various process parameters on edge shapes[4, 5, 6]. Spiegel et al. proposed three types of edge shapes to represent the global edge shapes[7].

On optimization, Passmore et al. performed surrogate modeling on coating thickness and roughness under various process variables[8]. However, this study did not consider edge shape optimization. Yoon et al. performed data-driven analysis on local edge shape metrics, but did not attempt to optimize the global edge shapes[6].

3. Methods and results

Our method quantifies global edge shape quality using a supervised classification model. The model estimates probabilistic scores for edge shape types, and computes the global quality by the Kullback-Leibler divergence from the ideal class probability distribution. Local edge shape quality is quantified using pre-defined metrics from previous studies. We provide a reproducible algorithm to compute these metrics from edge shape data. By combining these two types of qualities, we define a shape loss and construct its surrogate model, which is then used in Bayesian optimization to identify optimal process conditions. Finally, we propose integrating this framework with a self-driving laboratory platform for

autonomous discovery of optimal process conditions for industrial manufacturing.

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References

[1] T Dobroth and Lewis Erwin. Causes of edge beads in cast films. *Polymer Engineering & Science*, 26(7):462–467, 1986.

[2] Edgar B Gutoff and Edward D Cohen. *Coating and drying defects: troubleshooting operating problems*. John Wiley & Sons, 2006.

[3] Marcel Schmitt, Philip Scharfer, and Wilhelm Schabel. Slot die coating of lithium-ion battery electrodes: investigations on edge effect issues for stripe and pattern coatings. *Journal of Coatings Technology and Research*, 11(1):57–63, 2014.

[4] Boris Bitsch, Jens Dittmann, Marcel Schmitt, Philip Scharfer, Wilhelm Schabel, and Norbert Willenbacher. A novel slurry concept for the fabrication of lithium-ion battery electrodes with beneficial properties. *Journal of Power Sources*, 265:81–90, 2014.

[5] Sandro Spiegel, Alexander Hoffmann, Julian Klemens, Philip Scharfer, and Wilhelm Schabel. Optimization of edge quality in the slot-die coating process of high-capacity lithium-ion battery electrodes. *Energy Technology*, 11(5):2200684, 2023.

[6] Jihwan Yoon, Kyengmin Min, Jisoo Song, and Jaewook Nam. Controlling slot-coating edge profiles of battery electrodes. *ACS Applied Materials & Interfaces*, 2025.

[7] Sandro Spiegel, Thilo Heckmann, Andreas Altvater, Ralf Diehm, Philip Scharfer, and Wilhelm Schabel. Investigation of edge formation during the coating process of li-ion battery electrodes. *Journal of Coatings Technology and Research*, 19(1):121–130, 2022.

[8] Christopher Passmore, Kai E Wu, Jonathan R Howse, George Panoutsos, and Stephen J Ebbens. Surrogate-assisted optimization of roll-to-roll slot die coating. *Scientific Reports*, 15(1):29185, 2025.