Title: Easy Electrospinning: Towards Multimodal Generative Inverse Design of Electrospun Nanofibres Using Experimental Parameters and SEM-based Morphology Representations

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Abstract:

Electrospinning is a versatile technique for fabricating polymeric nanofibres and is widely used in biomaterials, tissue engineering, and related applications [1, 2]. However, obtaining fibres with desired diameters and morphologies remains challenging, as the process depends on complex and nonlinear interactions between solution properties, processing parameters, environmental conditions, and equipment-dependent factors. Consequently, experimental optimisation still relies largely on trial-and-error strategies, which are time-consuming and material-intensive. Although machine learning has increasingly been applied to electrospinning, most studies focus on forward prediction, typically estimating fibre diameter from a limited set of experimental parameters [3-6]. In practice, however, fibre fabrication often requires solving the inverse problem: identifying suitable experimental conditions from target fibre properties and environmental constraints.

In this work, we present an ongoing PhD project conducted within the framework of **PostGenAI@Paris**, an interdisciplinary and cross-sector consortium led by Sorbonne University through its **SCAI** cluster (Sorbonne Cluster for Artificial Intelligence). The project aims to develop a multimodal inverse design framework for PCL-based electrospinning. The long-term objective is to build a generative model capable of recommending experimental conditions that produce target fibre diameters and morphologies under given environmental conditions. To support this goal, we constructed a structured electrospinning dataset containing approximately 1,800 experimental records. The dataset focuses on a PCL/HFIP solution system and includes processing parameters, temperature, humidity, fibre diameter measurements, and corresponding SEM (scanning electron microscope) images. images. In parallel, we developed an internal electrospinning experiment data management system to standardise future data collection and support long-term dataset expansion within the laboratory.

A key contribution of this project is the integration of SEM image information into the analysis of electrospinning conditions. SEM images provide direct visual evidence of fibre formation and morphological defects that are not captured by scalar diameter-based metrics. We therefore use DINOv3 [7], a large vision model, as an off-the-shelf feature extractor for SEM images. From the extracted image features, we propose a Morphology Score Vector (MSV), which quantifies both the similarity of each SEM image to reference morphologies, ranging from droplets and droplet-fused fibres to fused fibres and fibres, and a continuous stage score capturing the transition from non-fibrous structures to well-formed fibrous networks, with fibre morphology corresponding to a balanced electrospinning system and therefore representing, in most cases, the desired outcome. Preliminary UMAP [8] visualisations show that enriching experimental and environmental parameters with MSV features produces a more structured representation space than using tabular parameters alone, suggesting that SEM-derived morphology information can complement fibre diameter measurement, providing a more comprehensive description of electrospinning outcomes.

Future work will focus on refining the dataset, evaluating conditioning strategies, and training diffusion- or flow-based generative models for inverse design. Key challenges include incorporating environmental constraints, defining suitable conditioning and guidance mechanisms, modelling conditional probability distributions tractably, and designing an effective interface for querying the AI system through structured parameters or natural language. Ultimately, this project aims to move towards an AI-assisted workflow that translates desired nanofibre characteristics into experimentally relevant electrospinning recommendations.

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