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Physics-Informed Neural Network for Bioprocess digitalization

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Abstract
Bioreactors are fundamental to bioprocess technology, yet the complexity of bioreactor systems continues to challenge effective digitalization and optimization. The intricate, dynamic nature of cell cultivation systems, affected by cell population heterogeneity, genetic instability, and intracellular regulatory mechanisms, poses a significant challenge for modeling and control. Mechanistic models based on first-principles equations mimic the system dynamics through known physical/ biological knowledge. However, they are often constrained by high mathematical complexity, extensive parameterization, identifiability problems, and high computational demand. In response to these limitations, hybrid mechanistic/machine learning approaches are gaining traction in bioprocess applications (Pinto et al., 2022). The hybrid model combines machine learning, e.g., feed forward neural networks (FFNN), with the mechanistic model, alleviating their limitations by incorporating prior knowledge into the model structure, thereby reducing data dependency and enabling more efficient process optimization.
Recently, Physics-Informed Neural Networks (PINN) have emerged as an alternative framework to embed physical laws (expressed through differential equations (ODEs or PDEs)) into neural network models via the training method. This ensures that the neural network models not only fit the available data but also adhere to the underlying governing laws of the system (Raissi et al., 2019). In this study, we propose a tandem FFNN PINN architecture to model a generic bioreactor system. The first network (FFNN-1) parameterizes the bioreactor state variables as a function of time and control inputs, whereas the second network (FFNN-2) parameterizes the reaction kinetics as a function of bioreactor state variables. The training of a PINN involves the simultaneous minimization of data and a physics loss function. The proposed tandem FFNN PINN structure enhances the training convergence and the ability of the model to capture complex nonlinear dynamics typical of bioreactor systems. The proposed PINN framework is benchmarked against a hybrid semiparametric model using several case studies, including a simple microbial logistic growth process and more complex fed-batch bioreactor problems. The models were trained on data from a single batch, and their extrapolation capability was evaluated across 14 testing batches without volume measurement during training, which were governed solely by embedded physical laws. Despite this demanding testing scenario, the PINN model demonstrated high predictive accuracy, achieving a coefficient of determination R2=0.99 for biomass and R2=0.98 for volume (Figure 1). This study shows that PINN are very efficient at capturing bioreactor dynamics with a very low number of data points, demonstrating their ability to generalize to unseen scenarios. There was, however, no definite evidence that PINN overcame hybrid semiparametric modeling for the problems addressed.

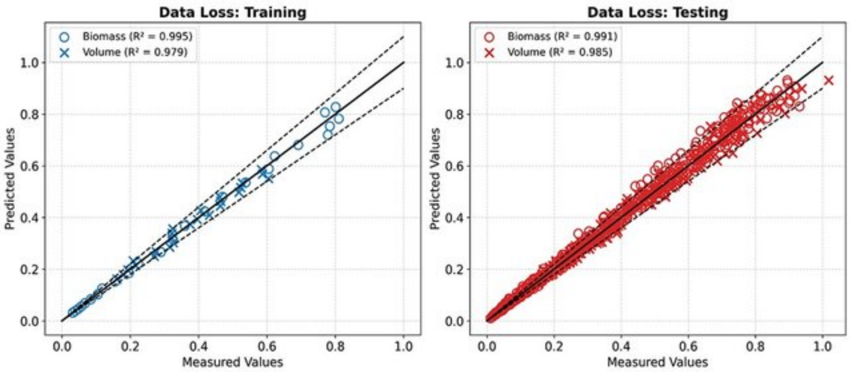

Figure 1: Prediction result

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