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Data driven modelling and optimisation of a batch reactor using bootstrap aggregated deep belief networks

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Batch reactors are suitable for the agile manufacturing of high value added products such as pharmaceuticals and specialty chemicals as the same reactors can be used to produce different products or different grades of products. Batch chemical reaction processes are typically highly nonlinear and batch to batch variations commonly exist in practice. Optimisation of batch process operation is essential for the enhanced production efficiency and product quality. Batch process optimisation usually requires an accurate process model that can accurately predict the end of batch product quality variables. Developing accurate mechanistic models for batch process is typical very time consuming and effort demanding. This is because a chemical reaction network usually involves a large number of reactions and some reaction pathways and/or kinetic parameters are not readily available. To overcome this difficulty, data-driven models developed from process operation and plant testing data should be capitalised. As batch chemical reaction processes are typically very nonlinear, nonlinear data-driven modelling techniques should be utilised.

Deep belief networks (DBN) has emerged as an efficient machine learning technique for developing nonlinear data-driven models and have shown superior performance compared to the conventional multi-layer feed-forward neural networks. However, the generalisation performance of DBN is still affected by the available modelling data and it is still quite difficult to build a perfect DBN model. To enhance the generalisation performance of DBN models, bootstrap aggregation of multiple DBN models is studied in this paper. Instead of building just one DBN model, several DBN models are developed from bootstrap re-sampling replication of the original modelling data and these DBN models are combined together to form a bootstrap aggregated DBN model (BAG-DBN). It is shown in this paper that the generalisation performance of BAG-DBN is significantly better that that of a DBN model. Furthermore, model prediction confidence bounds can be readily obtained from the individual DBN model predictions. The model prediction confidence bound can be incorporated into the batch reactor optimisation framework to enhance the reliability of the resulting optimal control policy. A simulated batch chemical reactor is used to demonstrate reliable data-driven modelling and optimisation using BAG-DBN.

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