On the assumption-free methodology for data-driven batch process monitoring

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Abstract

Conventional multivariate statistical techniques for batch process monitoring typically require uniform trajectory length for all measured variables across all batches. This can be achieved by data alignment, namely data equalization (all the variables are expressed at the same sampling rate across batches) and synchronization (all the landmarks for the variables trajectories are aligned in time across batches; González-Martínez *et al.*, 2018). However, advanced alignment techniques, such as dynamic time warping (Kassidas *et al.*, 1998) are computationally intensive and can generate artifacts, especially when some batches are significantly shorter than the chosen reference (González-Martínez *et al.*, 2014). The assumption-free monitoring technique (Westad *et al.*, 2005) is a promising alternative that overcomes the uniform-length limitation. However, design and implementation of this technique is challenging due to limited documentation available in the open literature.

In this study, we provide guidelines to streamline the design and implementation of an assumption-free process monitoring model. Furthermore, we introduce a methodology for fault diagnosis that enhances the standard T^2 contribution plot by more accurately identifying variables causing deviations from the common batch trajectory. We test the assumption-free monitoring methodology on five datasets. Results show that the assumption-free approach consistently outperforms a standard one based on batch-wise unfolded aligned trajectories of the process variables, especially when the number of time samples is large.

Keywords: batch processes; process monitoring; trajectory synchronization; PCA; principal component analysis

References

González-Martínez, J. M., Camacho, J., & Ferrer, A. (2018). MVBatch: A Matlab Toolbox for Batch Process Modeling and Monitoring. *Chemom. Intell. Lab. Sys.*, **183**, 122–133.

González-Martínez, J. M., de Noord, O. E., & Ferrer, A. (2014). Multisynchro: A Novel Approach for Batch Synchronization in Scenarios of Multiple Asynchronisms. *J. Chemom.*, **28**, 462–475

Kassidas, A., MacGregor, J. F., & Taylor, P. A. (1998). Synchronization of Batch Trajectories Using Dynamic Time Warping. *AIChE J.*, **44**, 864–875.

Westad, F., Gidskehaug, L., Swarbrick, B., & Flåten, G. R. (2015). Assumption free modeling and monitoring of batch processes. *Chemom. Intell. Lab. Sys.*, **149**, 66–72.