ISBN 13 978-952-5183-62-7

Mechanistic AI: physics-driven machine learning

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November 4, 2022

Traditional machine learning models are only able to describe phenomena captured in the training data of relatively high quality. Moreover, such models fall short when applied to a real process containing unmeasured disturbances, noise and unreliable sensing devices. In this work, we demonstrate a novel approach, Mechanistic AI, which provides robust models which not only generate accurate predictions, but also provide insights into the system beyond the information contained in the training data. Mechanistic AI is physics driven, where the skeleton of the model is based on first-principles: mass and energy conservation while data provides calibration for accurate predictions. Mechanistic AI does not require a detailed first-principle model but only a general level formulation of mass and energy conservation. This allows to predict measurable variables and estimate unmeasurable ones. Furthermore, the aforementioned skeleton regularizes any noise and inconsistencies present in the data, thus even low-quality data can be readily utilized by Mechanistic AI. Further, due to physics based frame, Mechanistic AI models can be easily generalized with only limited or no tailoring. In addition, Mechanistic AI model is constrained to produce valid results even on out-of-distribution data due to the inclusion of physics. In contrast to the Mechanistic AI, traditional supervised machine learning models are usually non-transferable to other units, have unknown validity limits, are difficult to interpret as well as cannot provide insight beyond information contained in training data. Summarizing, Mechanistic AI has unique features unattainable by traditional supervised ML models and can be applied in process control which requires robust models as well as in predictive and prescriptive maintenance which require deep insight into the system. In this work, we demonstrate the easiness of model formulation for Mechanistic AI and explore the implications of combining data and physics in a novel way to produce reliable prediction and estimation results.

Based on the obtained results, Mechanistic AI demonstrated the ability to not only predict process variables but also to estimate unmeasurable physical quantities. In terms of data efficiency and development time, our physics driven technique required significantly less data and development time compared to neural networks based approach which demanded 50 times more data and tedious architecture selection procedure to reach similar accuracy. In addition, our method was even able to reconciliate inconsistencies in training data, a result unattainable by any other approach. Applications of Mechanistic AI can provide estimates and predictions of many common phenomena in the process industry: heat transfer and fouling estimation, valve stiction assessment, estimation of reaction rate and intermediate concentrations and many others. Mechanistic AI models can be readily deployed using Scientia data platform as a central part of any control or analytics solution.