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Editorial: Hybrid modeling-blending physics with data

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Editorial on the Research Topic
Hybrid modeling-blending physics with data

Introduction

Physics-based modeling methods have been widely used in industrial applications, where the behavior of a system is derived from the first principles of the underlying physics. As the system becomes more complicated, acquiring an accurate solution, in the engineering sense, to a set of governing equations subjected to the associated boundary conditions gets more challenging and computationally expensive. On the other hand, the behavior of a system can also be determined through sensory observations of the input to and output from the system. Nonetheless, the predictability of the data-driven approximate model heavily depends on the volume and quality of the data based on which the model has been constructed, and the generalizability of the model is limited. A natural way of improving the predictability and generalizability of a model is to blend physics with data by utilizing the advantages of both, especially when sensors and computational resources are becoming increasingly available and affordable.

In this special Research Topic on hybrid modeling, five impactful papers are included. A summary of the studies is given below.

Summary of the studies

In the study by Song et al., a transfer function was developed to predict in a real time fashion the dynamic states (displacement and velocity) at the formation evaluation sensor of a logging while drilling (LWD) tool using the measured data at the motion sensor as the input. The unscented Kalman filter was used to fuse the dynamic first principals and the motion sensor data. The uncertainties induced by several sources including the gap size, bumper material, motion level, and sensor noise were quantified. The transfer function was validated first with synthetic data from a multi-scale finite element model and then with experimental data from an instrumented roll test. The developed model can be used to flag risks and optimize drilling operations to assure quality of real time answer products provided by the LWD tool.

Hafid et al. studied the crashworthiness of a thin-walled square steel tube containing an elliptical crush initiator. Numerical impact experiments were conducted with finite element simulations, the results of which were used to generate response surfaces. The established response surfaces were then employed to optimize the dimensions and location of the crush initiator with the objectives of minimizing the peak force and maximizing the mean crushing force, the crush force efficiency, and the specific energy absorption. The optimized solution was validated with finite element analysis to demonstrate a noticeable reduction in the peak force, a pronounced increase in the crush force efficiency, a moderate increase in the crush force efficiency, and a slight decrease in the specific energy absorption.

Kochan and Yang proposed a physically constrained Gaussian process regression model that was trained with the quantum-inspired Hamiltonian Monte Carlo (QHMC) algorithm. Two types of physical constraints, including inequality and monotonicity, were considered and the constraints were probabilistically enforced. An adaptive learning algorithm was adopted to better select the constraint points. A theoretical analysis confirmed the convergence of the QHMC algorithm and the probabilistic approach. The methods were applied to several optimization problems. It was shown that the soft-constrained QHMC is more advantageous over both truncated Gaussian and hard-constrained QHMC for inequality-constrained Gaussian processes with enhanced accuracy and efficiency, particularly for high-dimensionality problems. For monotonicity-constrained Gaussian processes, the QHMC-based algorithms outperform the additive Gaussian process method, particularly when noise and large datasets are involved, in terms of efficiency and variances.

In their study on graph time-series problems, Sun et al. proposed two physics-informed graph neural network architectures to address the learning challenges of having insufficient accuracy and robustness when the training and test data come from different circumstances. Physics was fused in the Reaction-Diffusion Graph Convolutional Network (RDGCN) by integrating differential equations for traffic speed evolution, and in the Susceptible-Infectious-Recovered Graph Convolutional Network (SIRGCN) by incorporating a disease propagation model in the graph neutral networks, respectively. The use of reliable and interpretable domain differential equations enables the models to be generalizable to unseen patterns. Experimental studies demonstrated superior efficiency and robustness of the models with mismatched test data over the state-of-the-art neutral network-based methods.

Walker et al. presented a variational autoencoder framework, named primaDAG, which is based on a Bayesian network model for extraction of dependent features from multimodal datasets with physical constraints enforced. A new parameterization scheme for directed acyclic graphs (DAGs) was introduced to learn the Bayesian network with an evidence-based lower-bound loss function. With a Gaussian mixture prior on the latent space, the model identifies the distribution of graph nodes, enabling feature discovery with conditional independence relationships. The efficacy of the primaDAG was demonstrated with a synthetic dataset and a real-world dataset of 3D-printted materials. The model was found able to disentangle data to extract interpretable dependent features during unsupervised learning.

Conclusion

Two common themes can be extracted from the five articles. First, digital approaches such as stochastic inference (Song et al.) and response surface method (Hafid et al.) were, respectively, used to optimize real time operation and design of a crush initiator. Sensory data was employed in the former, while synthetic data in the latter, mechanical engineering related applications. Second, physical constraints or differential equations were enforced onto a machine learning model to enhance efficiency and generalizability in supervised learning (Kochan and Yang; Sun et al.) and feature extraction in unsupervised learning (Walker et al.). The learning model was of classical type such as Gaussian process (Kochan and Yang) or of neural networks (Sun et al.; Walker et al.).

This Research Topic of articles sheds new light to the emerging trends of blending physics and data for better performance, efficiency, and/or robustness. It is our belief that hybrid modeling is gaining increasing popularity in broader applications and enhanced generalizability to datasets of various types, dimensions, and sizes.

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