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Data-Driven Model-Form Uncertainty with Bayesian Statistics and Neural Differential Equations

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Modeling real-world phenomena to any degree of accuracy is a challenge that the scientific research community has navigated since its foundation. Insufficient knowledge, such as inability to observe or represent all the relevant phenomena, induces uncertainty in the appropriate model form. Characterizing this model-form uncertainty (MFU) is essential to understanding the reliability of predictions made with these models, especially when such predictions inform high-consequence decisions. Here we present a novel model-form uncertainty representation which combines Bayesian statistics with Universal Differential Equations [1], a powerful new approach to data-driven modeling wherein a universal function approximator (a neural network in this work) is embedded within a known differential-equation model at the source of MFU. The neural network is endowed with a probabilistic representation and is updated using available observational data in a Bayesian framework. By representing the MFU explicitly and deploying an embedded, data-driven model, this approach enables an agile, expressive, and interpretable method for representing MFU.

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