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Physics-informed Machine Learning in Gaussian Process Regression

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Gaussian Process Regression (GPR) is a powerful interpolation technique to construct a predictive model with a finite set of observation points available in a system. The analytical property of GPR, wherein any linear transformation of a Gaussian process remains Gaussian, offers distinctive opportunities for integrating diverse forms of physics-based knowledge into the GPR framework. In this work, we propose three hybridization approaches that integrate physics-based knowledge with GPR, aiming to augment the GPR model's capacity to incorporate crucial physics-based insights and effectively bridge the gap between domain-specific knowledge and data-driven predictions. First, we address the impact of physics-based penalization in hyperparameter optimization of GPR. The hyperparameters in GPR are often estimated by maximum likelihood estimation (MLE), but it may produce biased estimates under sparse data scenarios as it solely depends on training data. To tackle this challenge, leveraging additional physics-based information available within the system to regularize MLE can yield a more refined hyperparameter set. This, in turn, enhances the predictive efficacy of the model by reducing the discrepancy with respect to physical information. We present a series of results showing that the physics-based penalization in MLE can improve prediction performance, reduce uncertainty, mitigate overfitting problems, and capture underlying physics that might remain undiscoverable using standard data-driven approaches. The incorporation of physics-based knowledge through the regularization process enhances the overall robustness and accuracy of the GPR model, making it well-suited for applications where sparse data and physics-based constraints coexist. Next, our attention is directed towards the commonly overlooked prior mean function in GPR modeling. Modelers often resort to employing a zero-prior mean, while inference predominantly relies on the kernel. However, we emphasize that both the prior mean and the kernel function are fundamental components of the Gaussian Process, and the model is fully defined by these two components. Upon thorough examination, we have discovered that the prior mean can play a crucial role in incorporating physics into the model. Through the incorporation of additional physical information alongside observation data, a meaningful physics-based prior mean can be constructed, effectively aligning the GPR model with underlying physics and leading to improved prediction performance. In this study, we utilize the Physics-informed Neural Network (PINN) to estimate the prior mean function. We select PINN for its advantageous overparameterized characteristics, facilitating efficient objective function minimization, and its seamless integration and hybridization with GPR through backpropagation, enabling the reformulation of various physical constraints. Lastly, we introduce a novel kernel in GPR that effectively incorporates various types of physical constraints inherent in the system. This new kernel, referred to as the physics-infused kernel, is devised by assessing the model's deviations from the established physical constraints at different input locations. By quantifying these violations within the system domain, we are able to rectify and fine-tune the covariance information between different outputs to align more closely with the underlying physics. The incorporation of this physics-infused kernel allows us to simultaneously consider both the data-fit and physics-fit of the model, resulting in a more comprehensive representation of the system. In different case studies with varying physical constraints, we show that the initially stationary data-based kernel can be transformed into a non-stationary kernel when integrated with physical information, and the true data structure can be discovered by effectively reconstructing the covariance information in the model.