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Gradient-Based Active Learning with Gaussian Processes for Global Sensitivity Analysis

In recent decades, numerical experimentation has established itself as a valuable and cost-effective alternative to traditional field trials for investigating physical phenomena and evaluating the environmental impact of human activities. Nevertheless, high-fidelity simulations often remain computationally prohibitive due to the detailed modelling required and the complexity of parameter selection. To overcome these challenges, surrogate models constructed from a limited number of complex model evaluations are commonly used to drastically reduce computational costs and quantify uncertainties. In this context, we propose an active learning approach that, for a fixed evaluation budget, intelligently reduce the dimension of the input space to optimize surrogate model performance.

Specifically, our methodology builds on new advances in active learning for sensitivity analysis—such as Sobol indices and Derivative-based Global Sensitivity Measures (DGSM)—by leveraging derivatives obtained from a Gaussian Process (GP) surrogate. The benefits of our approach are demonstrated through several case studies, ranging from synthetic benchmark functions to a real-world environmental application involving physically-based modelling of pesticide transfer. Our results highlight the potential of this strategy to enhance sensitivity analysis in computationally intensive modelling scenarios.

Special/ Invited session

Classification

Both methodology and application

Keywords

Active Learning, Gaussian Process, Sensitivity Analysis

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