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Multifidelity Gaussian process regression for solving nonlinear partial differential equations

Kernel-based methods provide a principled alternative to classical numerical solvers for nonlinear partial differential equations (PDEs), especially in mesh-free settings with built-in regularization and uncertainty quantification. Traditional discretization techniques such as finite differences or finite elements can become computationally demanding for nonlinear or multiscale problems. In contrast, the variational framework of Y. Chen et al. formulates PDE solving as a constrained minimization problem in a reproducing kernel Hilbert space (RKHS), with a natural Gaussian-process (GP) interpretation.

In this setting, the solution is defined as the minimizer of the RKHS norm subject to PDE and boundary constraints at collocation points. This formulation is equivalent to the maximum a posteriori estimator of a GP conditioned on the constraints, making the choice of kernel central to solution quality, regularity, and stability.

We introduce a multifidelity physics-informed methodology for constructing RKHSs adapted to PDE resolution. We assume access to low-fidelity simulations and sparse high-fidelity observations. From the low-fidelity observations, we estimate an empirical covariance and approximate it by a smooth kernel within a parametric family. High-fidelity information is incorporated using the autoregressive cokriging model of Kennedy and O'Hagan :

$$Y_H = \rho Y_L + Y_d.$$

The resulting RKHS is used directly in the PDE-constrained problem. We also extend the framework to non-centered GPs using a cokriging-informed mean. Numerical results on Burgers equations show reduced sensitivity to hyperparameters compared with single-fidelity approaches, while preserving the differentiability required by kernel-based solvers.

Special/ Invited session

Classification

Mainly methodology

Keywords

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