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Physics-informed Gaussian process regression : theory and applications

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Gaussian process regression (GPR) is the Bayesian formulation of kernel regression methods used in machine learning. This method may be used to treat regression problems stemming from physical models, the latter typically taking the form of partial differential equations (PDEs).

In this presentation, we study the question of the design of GPR methods, in relation with a target PDE model. We first provide several necessary and sufficient conditions describing how to rigorously impose certain physical constraints (explicitly, the distributional PDE constraint if the PDE is linear, and the control of the W^{m,p} Sobolev energy norm) on the realizations of a given Gaussian process. These results only involve the kernel of the Gaussian process.

We then provide a simple application test case, with the estimation of the solution of the 3D wave equation (central in acoustics), as well as the estimation of the physical parameters attached to this PDE. We finish with providing some outlooks concerning the design of finite difference schemes for solving PDEs, as well as the case of nonlinear PDEs.

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