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Prediction of physical fields under linear constraints

Metamodeling is a fundamental approach for approximating computationally expensive numerical simulations in engineering applications, such as uncertainty propagation and sensitivity analysis. In this work, we address the simultaneous prediction of multiple high-dimensional physical fields governed by linear equality constraints, a setting that arises naturally in problems involving conservation laws or incompressibility conditions. Gaussian Process (GP) regression is a natural tool for this task given its effectiveness in small sample regimes, but it faces two intertwined challenges: managing the high dimensionality of the discretized output fields, and enforcing the physical constraint in predictions. A common strategy to handle linear constraints consists in deducing one output from the others via the constraint relation, and building an unconstrained surrogate on the remaining fields. Through an extensive empirical benchmark, we show that this deductive approach suffers from a sensitivity to the arbitrary choice of which output to deduce, affecting both predictive accuracy and uncertainty quantification. To address these limitations, we propose first a specific PCA procedure for multi-field data, coined row-wise PCA, which has the interesting property of preserving the constraint in the latent space. Since standard PCA strategies for multi-field data (field-wise, column-wise) do not preserve such constraints, we investigate theoretically the optimality of the row-wise choice and provide conditions under which it incurs a negligible reconstruction cost. In a second step, we consider a linearly-constrained multi-output GP approach based on a specific kernel parametrization. The proposed framework is validated on a population dynamics problem and on an industrial computational fluid dynamics application, which involves the prediction of Reynolds stress tensor components under the incompressibility constraint. We demonstrate competitive predictive performance while guaranteeing strict constraint satisfaction.

Special/ Invited session

Classification

Both methodology and application

Keywords

Gaussian process, PCA, linear constraints

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Track Classification: Uncertainty quantification and computer experiments