Gradient-enhanced surrogate modelling and sensitivity analysis with chaos expansions

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To surrogate expensive computer simulations and calculate Sobol' sensitivity indices, sparse regression-based polynomial chaos expansions are a well-known tool. They represent the model in a basis of multivariate polynomials which are orthogonal with respect to the distribution of the input parameters. Recently, another type of chaos has been proposed, whose basis consists of the eigenfunctions of an associated Sturm-Liouville equation [1,2,3], see Fig. 1 for an illustration. The advantage of this basis is that by construction, the partial derivatives of the basis form again a basis which is orthogonal with respect to the same distribution as the original basis. This makes it possible to use model derivatives, if available, for the surrogate, while keeping advantageous orthogonality properties of the regression matrix.

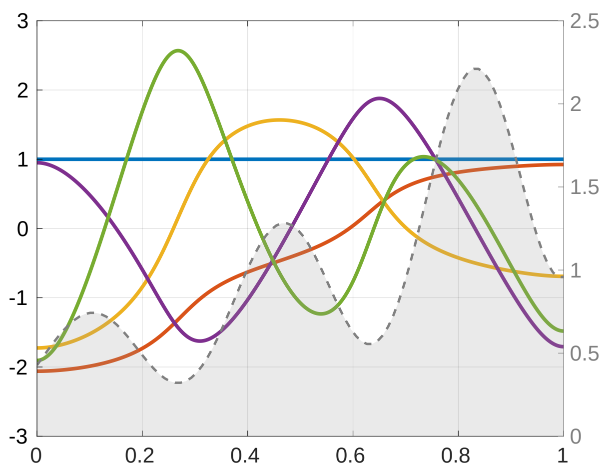

Figure 1: Illustration of the first five eigenfunctions of a one-dimensional Poincaré basis for a distribution with three modes (visualized by the gray area with y-scale on the right-hand side of the plot)

In our previous work [2], we used sparse regression-based Poincaré chaos expansions to compute surrogate models and sensitivity indices (Sobol' indices and DGSM) from model evaluations and derivatives separately. We found that while the Poincaré methodology did not outperform PCE as a surrogate model in our experiments, the Sobol' indices computed through derivative-based Poincaré expansions seem to be an efficient screening tool.

However, we did not yet built surrogates from both model evaluations and derivative values at once. This problem has been analyzed by Adcock and Sui (2019) [3]. They have shown that by applying weighted ℓ^1 regression to gradient-augmented data, the surrogate converges in a stronger norm than for model evaluations alone, with an equivalent number of model (resp. gradient) evaluations.

In this contribution, we provide an all-included methodology for gradient-augmented analysis which combines model evaluations and derivatives in the two main stages of surrogate modeling and global sensitivity analysis. First, we further examine the gradient-augmented regression problem by handling different orders of magnitude for model evaluations and partial derivatives. Second, we present a new estimator for Sobol' indices which uses both model evaluations and derivative values. It is built as a minimal-variance aggregation of estimators computed from chaos expansions and is particularly well suited for screening. We demonstrate the performance of the methodology on a hydrological problem where gradients are available via the adjoint method.

References:

[1] O. Roustant, F. Gamboa and B. Iooss, "Parseval inequalities and lower bounds for variance-based sensitivity indices", *Electronic Journal of Statistics*, **14**(1):386–412, 2020.

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[3] B. Adcock and Y. Sui, "Compressive Hermite Interpolation: Sparse, high-dimensional approximation from gradient-augmented measurements", *Constructive Approximation*, **50**(1):167–207, 2019.

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