Non-Intrusive Uncertainty Quantification with Polynomial Chaos Approximations for a Stochastic Stern-Gerlach Magnet Model

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In the context of uncertainty quantification for electrical devices, polynomial chaos methods are known to provide fast and accurate results. Sparse approximations are employed for problems characterized by high dimensional uncertainty. Non-intrusive computation of surrogate models may employ interpolation, projection or regression schemes. The choice of method is critical in the case of computationally demanding models, e.g. finite element magnet models, where accurate results must be achieved with a minimum number of model evaluations. The present paper considers the ordinary least squares and least angle regression methods, applied to a stochastic Stern-Gerlach magnet model. Results regarding surrogate model accuracy and computational costs are presented.

Index Terms—Least angle regression, least squares collocation, polynomial chaos, Stern-Gerlach magnet, uncertainty quantification

I. INTRODUCTION

Due to fabrication imperfections, electrical devices deviate from their specifications, e.g. with respect to their geometrical characteristics. These uncertainties cannot be avoided even for highly specialized devices, such as Stern-Gerlach magnets used in physics research [4], and can affect output quantities of interest (QoI) of the device. However, their impact on QoI can be quantified by computing statistical measures (e.g. moments, sensitivity indices) as part of the simulations undertaken during the device's design phase.

Polynomial chaos (PC) [11] approximations based on ordinary least squares (OLS) regression [7] can provide accurate results and reliable surrogate models with few model evaluations, when a low number of uncertainties is considered. Problems featuring a large number of uncertain parameters must be dealt with sparse approximations, like the least angle regression (LAR) [5] method. While quite successful, see e.g. [8], LAR is rarely encountered in the context of electromagnetics. In this work, both OLS and LAR are applied to a Stern-Gerlach magnet model with 10 input random variables (RVs).

II. NON-INTRUSIVE POLYNOMIAL CHAOS

Non-intrusive PC uses a fixed set of model evaluations to approximate a QoI with the polynomial chaos expansion (PCE)

$$\mathcal{Q}\left(\mathbf{y}\right) \approx \widetilde{\mathcal{Q}}\left(\mathbf{y}\right) = \sum_{k=1}^{K} \beta_k \Psi_k\left(\mathbf{y}\right), \tag{1}$$

where β_k are scalar coefficients and Ψ_k are multivariate polynomials, orthonormal w.r.t. the joint probability density function (PDF) of the independent RVs $\mathbf{Y} = (Y_1, \ldots, Y_N)$ [11]. Assuming a total degree basis with maximum polynomial order P, the number of PCE terms is $K = (P+N)!/(P!N!)$.

The OLS collocation method [7] computes coefficients β_k by solving the minimization problem

$$\hat{\beta} = \arg\min_{\beta} \sum_{m=1}^{M} \left(\mathcal{Q}\left(\mathbf{y}^{(m)}\right) - \widetilde{\mathcal{Q}}\left(\mathbf{y}^{(m)}\right) \right)^2. \tag{2}$$

Problem (2) is well-conditioned if the number of model evaluations is $M = cK$, with $c > 1$ being a sampling coefficient. Typical choices are $c = 2, 3$ [7]. Since the Smolyak sparse quadrature [1] schemes employed by spectral projection [6] or stochastic collocation [10] result in $M \approx 2^P N^P / P!$, OLS collocation's computational costs are lower for the same number of terms K. For a comparison, see Fig. 2. While a comparison on approximation errors versus collocation points is not presented, in Section IV we show that OLS yields acceptable approximation errors, hence the choice of method is justified.

Sparse approximations, i.e. with a few non-zero coefficients β_k, can be derived with the LAR method, even for $M < K$. Hence, LAR is especially well suited for cases where a large number of RVs is present, exactly because of the increase in approximation terms K. The LAR algorithm reads as follows:

1) Set all coefficients to zero. Set residual $\mathbf{r}$ equal to the vector of model evaluations $\mathbf{q}_M$.
2) Find polynomials $\mathbf{\Psi}$ most correlated to the current residual.
3) Estimate corresponding coefficients $\boldsymbol{\beta}$ with OLS.
4) Compute new residual $\mathbf{r} = \mathbf{r} - \gamma \boldsymbol{\beta} \mathbf{\Psi}$, where γ is a descent direction coefficient.
5) Repeat steps (2)-(4) until $\min(K, M-1)$ coefficients have been computed or until the residual change is insignificant.

For $M > K$, the OLS solution is computed.

III. STOCHASTIC STERN-GERLACH MAGNET MODEL

We consider the Stern-Gerlach magnet model from [9]. The geometrical degrees of freedom (DoF), i.e. x-y coordinates and weights of the control points which describe the geometry of the magnet's pole region (see Fig. **??**), are now introduced as independent and uniformly distributed RVs.

As QoI we consider the output of the optimization cost function

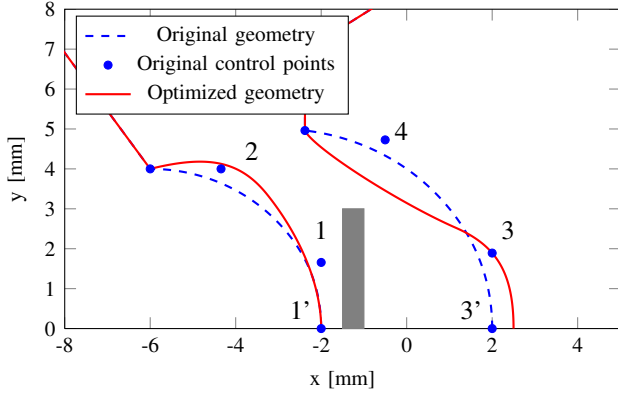$$\mathcal{Q} = \frac{\tau_w}{|\tau_{\text{avg}}|} + \epsilon - \frac{\tau_w}{|\tau_{\text{avg}}|}\epsilon, \tag{3}$$

Fig. 1. Original and optimized geometry of the Stern-Gerlach magnet's pole region, described by the control points 1–4 [9].

Fig. 3. Model evaluations vs relative leave-one-out (LOO) error.

introduced in [9], with τ_{avg} being the average magnetic field gradient, ϵ its inhomogeneity and τ_w a weighting factor.

IV. NUMERICAL RESULTS

An in-house MATLAB-based software was used for the deterministic magnet model. The Python library OpenTURNS [2] was used for the regression-based UQ analysis.

Fig. 2 presents the number of model evaluations M for different polynomial orders P and sampling coefficients c. For reasons of comparison, the corresponding number of evaluations needed for the Smolyak projection method is also presented. Again, note that a complete study should also include an accuracy-versus-evaluations comparison. This is an ongoing work and will be part of the full paper.

Regarding the accuracy of the PC approximation, Fig. 3 presents the relative leave-one-out error $\varepsilon_{\mathrm{LOO}}$ [3] w.r.t. M, corresponding to $P \in \{2, 3, 4\}$ and $c \in \{0.5, 0.8, 1, 2, 3, 5\}$. Error $\varepsilon_{\mathrm{LOO}}$ is chosen due to its reduced sensitivity to overfitting phenomena. It is defined as

$$\varepsilon_{\mathrm{LOO}} = \frac{\frac{1}{M} \sum_{m=1}^{M} \left(\mathcal{Q}\left(\mathbf{y}^{(m)}\right) - \widetilde{\mathcal{Q}}_{-m}\left(\mathbf{y}^{(m)}\right) \right)^2}{\mathrm{var}\left[\mathbf{q}_M\right]}, \quad (4)$$

where $\widetilde{\mathcal{Q}}_{-m}$ is the surrogate model built without the m-th collocation point. It can be observed that accurate enough surrogate models can be built with only a few available evaluations. Accuracy increases with the polynomial order and with the number of available model evaluations, as expected. Surrogate models which satisfy the desired accuracy demands can then be employed for otherwise computationally expensive studies, e.g. sensitivity analyses.

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Fig. 2. Model evaluations vs maximum polynomial order for 10 RVs.