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On the Choice of Design Points for Least Square Polynomial Approximations with Application to Uncertainty Quantification

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Abstract. In this work, we concern with the numerical comparison between different kinds of design points in least square (LS) approach on polynomial spaces. Such a topic is motivated by uncertainty quantification (UQ). Three kinds of design points are considered, which are the Sparse Grid (SG) points, the Monte Carlo (MC) points and the Quasi Monte Carlo (QMC) points. We focus on three aspects during the comparison: (i) the convergence properties; (ii) the stability, i.e. the properties of the resulting condition number of the design matrix; (iii) the robustness when numerical noises are present in function values. Several classical high dimensional functions together with a random ODE model are tested. It is shown numerically that (i) neither the MC sampling nor the QMC sampling introduce the low convergence rate, namely, the approach achieves high order convergence rate for all cases provided that the underlying functions admit certain regularity and enough design points are used; (ii)The use of SG points admits better convergence properties only for very low dimensional problems (say $d \leq 2$); (iii)The QMC points, being deterministic, seem to be a good choice for higher dimensional problems not only for better convergence properties but also in the stability point of view.

AMS subject classifications: 65C20, 65M70

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1 Introduction

In recent years, there has been a growing need for including uncertainty in mathematical models and quantify its effect on given outputs of interest used in decision making. In

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general, a probabilistic setting can be used to include these uncertainties in mathematical models. In such framework, the input data are modeled as random variables, or more generally, as random fields with a given correlation structure. Thus, the goal of the mathematical and computational analysis becomes the prediction of statistical moments of the solution or statistics of some quantities of physical interest of the solution, given the probability distribution of the input random data. Examples of quantities of interest could be the mean or the variance of the exact solution, the solution values in a given region, etc. This is the so called Uncertainty Quantification (UQ).

A fundamental problems in UQ is to approximate a multivariate function $Z = f(x,Y_1,Y_2,\cdots,Y_N)$ with random parameters $\{Y_i\}_{i=1}^N$, which might be a solution resulting from a stochastic PDE problem or other complex models. Stochastic modeling methods for uncertainty quantification are being well developed in recent years. A traditional approach is the Monte Carlo (MC) method [7]. In MC method, one first generates a number of random realizations for the prescribed random inputs and then utilizes existing deterministic solvers for each realization. Although the convergence rate of Monte Carlo method is relatively slow (converges asymptotically at a rate of $\frac{1}{\sqrt{K}}$ with K realizations), it is independent of the dimensionality of the random space, i.e., independent of the number of random variables used to characterize the random inputs. Significant advances have been made in improving the efficiency of Monte Carlo schemes during the past years. Stochastic collocation (SC) [17,18,23,24] method is another non-intrusive method. Like MC method, the SC method can be easily implemented and leads naturally to the solution of uncoupled deterministic problems, even in presence of input data which depend nonlinearly on the driving random variables. When the number of input random variables is small, the SC method is a very effective numerical tool. However, in many cases, a large number of collocation points are still needed to get a good convergence rate.

One of the most popular intrusive methods is the generalized polynomial chaos (gPC) methods [10,25], which are the generalizations of the Wiener-Hermite polynomial chaos expansion developed in [22]. Compared to the SC method, the gPC methods need relatively smaller number of degree of freedom, and such methods also exhibit fast convergence rates with increasing order of the expansions, provided that solutions are sufficiently smooth with respect to the random variables. However, the resulting set of deterministic equations is often coupled, thus, care is needed to design efficient and robust solver, and furthermore, the form of the resulting equations can become very complicated if the underlying differential equations have nontrivial and nonlinear forms [2,28].

To efficiently build such a gPC approximation, we consider in this work the lease square projection onto the polynomial spaces. The LS approach is actually a combination of the SC method and gPC method. It sakes a polynomial approximation for the unknown solution while using collocation points to evaluate the expansion coefficients. Such an idea has been used by many researchers and been given several different names [1,5,6,12,13], to name a few. To assure the well-posedness, the number of samples drawn from the input distribution is typically taken to be 2 to 3 times the dimension of the polynomial space.