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APPLICATION OF FINITE ELEMENT, GLOBAL POLYNOMIAL, AND KRIGING RESPONSE SURFACES IN PROGRESSIVE LATTICE SAMPLING DESIGNS

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Large-scale optimization and uncertainty analyses are often made feasible through the use of response surfaces as surrogates for computational models that may not be directly employable because of prohibitive expense and/or noise properties and/or coupling difficulties in multidisciplinary analysis.

This paper examines the modeling accuracy of piecewise finite-element interpolation, kriging, and polynomial regression used in conjunction with the Progressive Lattice Sampling (PLS) incremental design-of-experiments sampling approach. PLS is a paradigm for sampling a deterministic hypercubic parameter space by placing and incrementally adding samples in a manner intended to maximally reduce lack of knowledge in the parameter space. When combined with suitable interpolation methods, PLS is a formulation for progressive construction of response surface approximations (RSA) in which the RSA are efficiently upgradable, and upon upgrading, offer convergence information essential in estimating error introduced by the use of RSA in the problem.

The three PLS-compatible interpolation methods above were examined for performance in replicating a multimodal analytic test function as measured by several different indicators. Under relatively sparce sampling low-order polynomial approximations generally performed better than kriging interpolation. However, ultimately for the most dense sampling tried (PLS Level 7 having 41 samples over the 2-D parameter space), kriging matched the test function best. Finite-element interpolation (FE) performed almost as well as kriging under the most dense sampling and generally performed better under sparcer sampling. Polynomial regression (PR) also performed well, generally improving the fit of global polynmial RSA to the test function as samples were added. On balance, however, FE and kriging performed better than PR for the same number of samples, as conformability to the target function is limited by the orders of the terms in the regression polynomial, and these cannot be allowed too high or the polynomial can exhibit spurious oscillations away from the data points. Thus, it appears that PR may be less amenable than are kriging and FE to fitting general higher-order functions under dense sampling in the PLS framework.

Many more [diverse and higher-dimensional] functions must be tested before more firm conclusions can be drawn about the relative applicability of these interpolators under PLS. The process described in the paper provides a framework for future studies using other interpolation schemes, test functions, and measures of approximation quality.

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APPLICATION OF FINITE ELEMENT, GLOBAL POLYNOMIAL, AND KRIGING RESPONSE SURFACES IN PROGRESSIVE LATTICE SAMPLING DESIGNS

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Abstract

This paper examines the modeling accuracy of finite element interpolation, kriging, and polynomial regression used in conjunction with the Progressive Lattice Sampling (PLS) incremental design-of-experiments approach. PLS is a paradigm for sampling a deterministic hypercubic parameter space by placing and incrementally adding samples in a manner intended to maximally reduce lack of knowledge in the parameter space. When combined with suitable interpolation methods, PLS is a formulation for progressive construction of response surface approximations (RSA) in which the RSA are efficiently upgradable, and upon upgrading, offer convergence information essential in estimating error introduced by the use of RSA in the problem. The three interpolation methods tried here are examined for perfomance in replicating an analytic test function as measured by several different indicators. The process described here provides a framework for future studies using other interpolation schemes, test functions, and measures of approximation quality.

Introduction

Large-scale optimization and uncertainty analyses are often made feasible through the use of response surfaces as surrogates for computational models that may not be directly employable because of prohibitive expense and/or noise properties and/or coupling difficulties in multidisciplinary analysis. Examples of response surface usage to facilitate large-scale optimization and uncertainty analyses are cited in Romero (1998), Roux *et al.* (1996), Unal *et al.* (1996), and Venter *et al.* (1996).

For this study it is assumed that: 1) the computer model is expensive to evaluate; 2) the parameter space is a unit hypercube or can be accurately and inexpensively mapped into one; 3) the sampled or "target" function is a continuous, deterministic function over the parameter space; 4) reasonably general, arbitrary target functions are to be fitted; and 5) approximate response values are desired over the entire parameter space –*i.e.*, for global optimization or globally mapping inputs to outputs as might occur in sampling the parameter space for probabilistic information.

Given these specifications, the Progressive Lattice Sampling (PLS) incremental sampling design is invoked here that is in some sense optimal in reducing ignorance in the parameter space per each new sample added.† "Progressive" incremental sampling results in eventual convergence of a compatible response surface approximation to the target function being approximated. An assessment of the convergence state is essential in quantifying and limiting uncertainties arising from using response surface approximations in

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†In this context, reducing lack of knowledge implies a different sampling strategy than does knowledge maximization. PLS builds knowledge while reducing knowledge deficit but does not attempt to build *specific* or *targeted* knowledge in the manner of "adaptive" or "targeted" or "directed" sampling, which are used for efficient knowledge maximization. Thus, the PLS designs select sample locations strictly on geometric principles such that each new sample is "maximally far" from all other existing samples in the parameter space so that uniformity of coverage is maximized in the scheme.

"meta procedures" such as optimization and reliability analysis (Romero, 2000). The progressivity of PLS is also thought to be globally optimal in that, as samples are added in attaining each new Lattice Sampling "Level", all previous samples are fully leveraged with no redundancy or marginalization, and the spacing of samples throughout the parameter space remains maximized at all Levels.

Romero and Bankston (1998) examined the convergence properties of PLS using finite-element interpolation and found high Level-wise rates of convergence of calculated probabilities as the response surfaces were upgraded from Level to Level. In this paper, polynomial regression and kriging interpolation methods, which are also amenable to upgrading in incremental PLS, are also examined for performance on one of the test functions (Function #1) with respect to several different indicators of approximation quality.

Progressive Lattice Sampling "Incremental" Experimental Design

As presented here, the implementation of PLS has changed somewhat since it was first introduced by Romero and Bankston in 1998, but the essence is still the same.

Figure 1 illustrates the PLS plan in two dimensions. Level 1 consists of three samples illustratively located as shown. The sample at the center of the parameter space is fundamental. Assuming no *a priori* knowledge of the target function exists, the two other samples are located at arbitrarily picked mid-edges of the square. If enough is known of the target function to provide a basis and/or the response surface is to be used for probability/uncertainty analysis, then the mid-edges of the hypercube are picked that best suit the presiding conditions (Romero, 2000). For the present study there are no asymmetries in the applicable p.d.f.s, and no previous knowledge of the fitted function is interjected, so the two mid-edges to be sampled in the figure were arbitrarily selected. In n dimensions, Level 1 requires n+1 samples.

Lattice Sampling Level 2 adds n samples to complete a $2n$+1 layout exemplified in 2-D in the figure. Level 3 superposes a 2^n factorial design. Below 5 dimensions this corresponds to a face-centered central composite design. Level 4 superposes a Box-Behnken design to arrive at a 3^n full factorial design. (In two dimensions, Levels 3 and 4 turn out to be identical.) Level 5 adds a sub-scaled 2^n factorial design as illustrated in the figure. Level 6 adds the appropriate samples to complete a 5^n full factorial design, and Level 7 adds a sub-scaled 4^n full factorial design as shown.

Level 4 requires 81 samples for n=4 dimensions, 243 for n=5, and 729 for n=6. Level 7 requires 41 samples for n=2, 189 for n=3, and 881 for n=4. Though surmised to be an optimally efficient *progressive* sampling design, PLS becomes increasingly expensive with dimension and with Level attained. When affordable, PLS provides an efficient manner to, if not actually achieve convergence of quantities calculated from the response surface approximations, at least quantitatively estimate approximation-error magnitudes. Progressing through the first three PLS Levels for such an estimate can be done for n=5 dimensions with 43 samples, for n=7 with 143 samples, and for n=9 with 531 samples.

Some PLS-Compatible Interpolation Schemes

Compatible PLS interpolation schemes to be examined here are kriging, global polynomial interpolation, and piecewise finite-element interpolation.

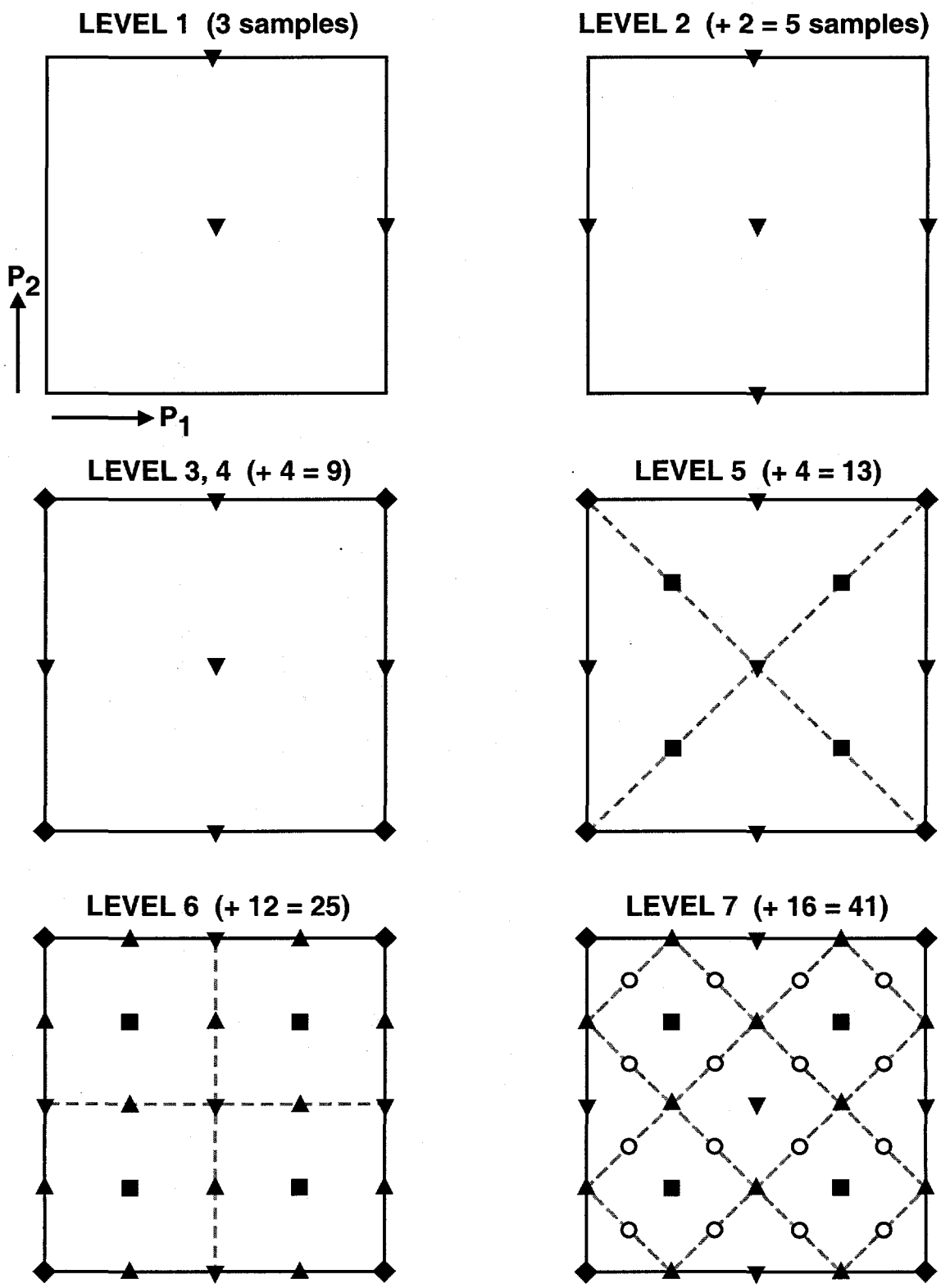

Figure 1. 2-D Progressive Lattice Sampling Design.

Kriging is a class of globally smooth function approximation methods developed in the fields of spatial statistics and geostatistics (Cressie, 1991). In the specific variant of kriging used in this study, the value of the interpolation function is strongly affected by sampled data that are near in the parameter space and weakly affected by data points that are farther away, according to directional spatial correlation parameters determined by maximum likelihood estimation. Another characteristic of the kriging method used in this study is that it reverts to the mean value of the sample data when used in extrapolation outside of the sampled data set. For more information on the kriging methods used here, see the works of Sacks *et al.* (1989), Koehler and Owen (1996), and Giunta and Watson (1998).

"Saturated" global polynomial approximations exactly match the number of ascending monomials or "terms" in the polynomial (beginning with the constant term) to the number of sample points in the parameter space, where the sample points are located such that all monomial coefficients can be accurately resolved. Such saturated polynomials pass through all sample points exactly. Examples of such approximations are a hyperplanar[‡] approximation based on the n+1 sample points in Level 1, a "simple" quadratic[**] approximation based on the $2n$+1 sample points in Level 2, and a full quadratic polynomial having 3^n terms for Level 4 (and for Level 3 in 2-D).

Though a polynomial of sufficiently high order can always be found to pass through all data samples in a deterministic parameter space, as the number of data points increases such saturated polynomial approximations increasingly tend to exhibit oscillation or "wiggliness" between the data points. Thus, as more samples are added, these types of approximations may not converge pointwise over the parameter space to the modeled function even though the approximations are exact at the sample points. Therefore, when working with global polynomial approximations, the order of the polynomial is generally limited to quadratic or cubic; and when the number of sample points exceeds the number of terms in the polynomial, regression is used to determine the monomial coefficients that make the polynomial best fit the data in a least-squares sense. Accordingly, regression is applied in the 2-D example below to best fit the 13-sample Level 5 data with a 9-term full quadratic polynomial and to fit the 25-sample Level 6 data and the 41-sample Level 7 data with a 16-term full cubic polynomial. All monomial terms in these polynomials were retained in this work, though under some conditions this is not desirable. (Methods such as "stepwise regression" (Venter *et al.*, 1996) exist to find a quasi-optimal subset of monomials.)

Saturated polynomial approximations are used in the finite-element modeling literature to represent function behavior on a local scale. Assemblages of these local approximations provide global approximations with good local conformance properties. Continuous, piecewise-smooth global approximations result with low-order-polynomial local variation. Example finite element interpolations are suggested in Figure 1, where Levels 5, 6, and 7 show parameter space discretizations into triangular and quadrilateral finite elements of up to quadratic order (Romero *et al.*, 1998). These globally C^0-continuous approximations are the only interpolants applied here that do not have continuity of first-order derivatives over the parameter space. This can inhibit their performance in optimization; however this is circumvented in the Finite-Element/Structured-Sampling "FESS" optimization scheme (Romero, 1999) that has proven to be more robust and efficient than classical and contemporary methods on a difficult 2-D noisy global optimization problem.

[‡]A hyperplanar response surface is linear in the set of all the input variables $\{x_i\} : f(\{x_i\}) = a_0 + \sum a_i x_i$.

[**]A simple quadratic response surface has the form: $f(\{x_i\}) = a_0 + \sum a_i x_i + \sum b_i x_i^2$.

Application Problem

Figure 2 plots the 2-D target function used in this study. This multimodal function is defined as:

$$\text{response}(p1,p2)=\left[0.8r+0.35\sin\left(2.4\pi\frac{r}{\sqrt{2}}\right)\right][1.5\sin(1.3\theta)]$$

on the domain $0 \le p1, p2 \le 1$,

where $r = \sqrt{(p1)^2+(p2)^2}$, $\theta = \text{atan}\left(\frac{p2}{p1}\right)$.

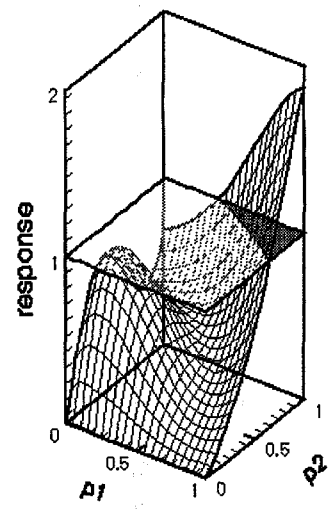

Figure 2.

Exact values (samples) of this function are obtained at the indicated Lattice points in Figure 1, and the data at the various Levels is then fitted and interpolated with kriging, saturated and regression polynomials, and piecewise finite element methods as applicable. At each Level, two measures of quality of the various interpolations are used: 1) average absolute error = [the sum of the absolute differences between exact and interpolated values of the target function at 441 equally space points on a 21x21 square grid over the domain]/[441]; and 2) calculated probability of exceedence of the 1.0 threshold plane in Figure 2 by Monte Carlo sampling of the approximations 10^6 times according to the joint normal probability density function (p.d.f.) described in (Romero *et al.*, 1998). As explained there, this approximates the integral of the joint p.d.f. over the exceedence region of the parameter space (shaded portion of the threshold plane) where the function exceeds the stipulated threshold value. This is representative of a reliability problem. This metric tests the ability of the approximation to reproduce the shape of the shaded region.

Results and Discussion

Figure 3 shows reduction of average absolute error for the various interpolation methods as the Lattice Levels are advanced through. Figure 4 shows convergence of the calculated probabilities to the "exact" probability of 0.007560 obtained by sampling the exact function at the 10^6 points in the parameter space. As in (Romero *et al.*, 1998), behaviors at thresholds of 0.2, 0.5, and 1.5 were also examined, and are not presented here for lack of room but will be presented at the conference and are fully considered in the following.

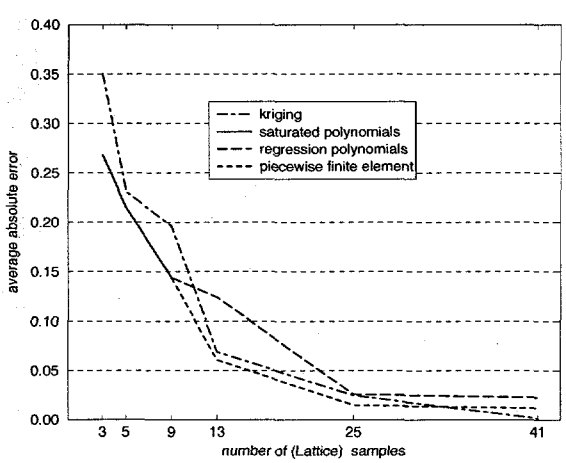

Figure 3. Level-wise convergence of average absolute error.

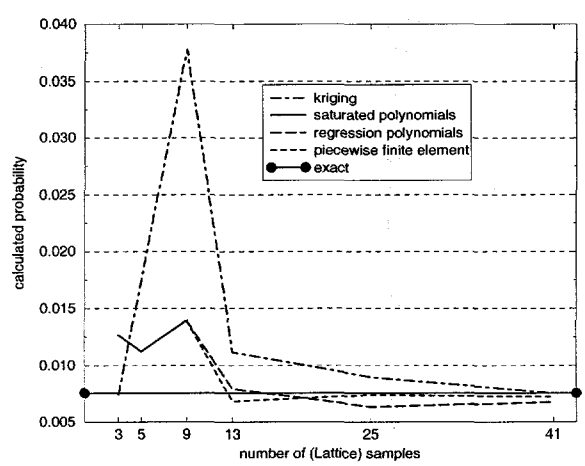

Figure 4. Level-wise convergence of calculated exceedence prob.

Only kriging and saturated polynomial approximations are applied at Levels 1, 2, and 3\4 here. At these lower Levels the low-order polynomial approximations generally perform better than kriging over the five cases studied (global average absolute error and four different exceedence thresholds). Kriging tended to be relatively unstable under sparse sampling (up Level 4). However, as is typical of most numerical systems, no methods tried here exhibited unbroken monotonic convergence as samples were added. At Levels 5, 6, and 7, kriging, polynomial regression (PR), and piecewise finite element (FE) interpolations were applied. At Level 5, PR was sometimes superior to FE over the five cases. Beyond Level 5, FE always performed better. At Level 5, kriging yielded perhaps the best average performance. At Level 6, FE always performed the best, with PR and kriging trading second and third over the five cases. Ultimately, at Level 7 kriging performed best, converging essentially to exact results in all cases. FE performed almost as well at Level 7, with the performance of PR generally leveling off after Level 6, after which the conformance of the cubic polynomial could not be significantly improved by adding more samples. Though many more [diverse and higher-dimensional] functions must be tested before more firm conclusions can be drawn about the relative applicability of these interpolators under PLS, this paper demonstrates the framework and process for future studies.

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