Design Science

Quadrature as applied to computer models for robust design: theoretical and empirical assessment

Daniel D. Frey[1], Yiben Lin[2] and Petra Heijnen[3]

1 *MIT, Department of Mechanical Engineering, Cambridge, MA, USA*
2 *Morgan Stanley, New York, NY, USA*
3 *Delft University of Technology, Technology Policy and Management, Delft, Netherlands*

Abstract

This paper develops theoretical foundations for extending Gauss–Hermite quadrature to robust design with computer experiments. When the proposed method is applied with m noise variables, the method requires $4m + 1$ function evaluations. For situations in which the polynomial response is separable, this paper proves that the method gives exact transmitted variance if the response is a fourth-order separable polynomial response. It is also proven that the relative error mean and variance of the method decrease with the dimensionality m if the response is separable. To further assess the proposed method, a probability model based on the effect hierarchy principle is used to generate sets of polynomial response functions. For typical populations of problems, it is shown that the proposed method has less than 5% error in 90% of cases. Simulations of five engineering systems were developed and, given parametric alternatives within each case study, a total of 12 case studies were conducted. A comparison is made between the cumulative density function for the hierarchical probability models and a corresponding distribution function for case studies. The data from the case-based evaluations are generally consistent with the results from the model-based evaluation.

Keywords: Robust design, uncertainty quantification, design of computer experiments

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Corresponding author
D. D. Frey
danfrey@MIT.EDU

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1. Introduction: the context in design

Robust parameter design is an off-line quality control method whose purpose is to reduce the variability in performance of products and processes in the face of uncontrollable variations in the environment, manufacture, internal degradation and usage conditions (Taguchi 1987; Phadke 1989; Wu & Hamada 2000). The variables that affect a product's response are classified into control factors whose nominal settings can be specified and noise factors that cause unwanted variations in the system response. In robust design, the space of control factors is searched to seek settings that are less sensitive to the noise factors and therefore exhibit less variation in performance.

Robust parameter design is increasingly performed using computer models of the product or process rather than laboratory experiments. Computer models can provide significant advantages in cost and speed of the robustness optimization process. Although random variations in noise factors can be simulated in a computer, the results of computer models generally lack pure experimental error

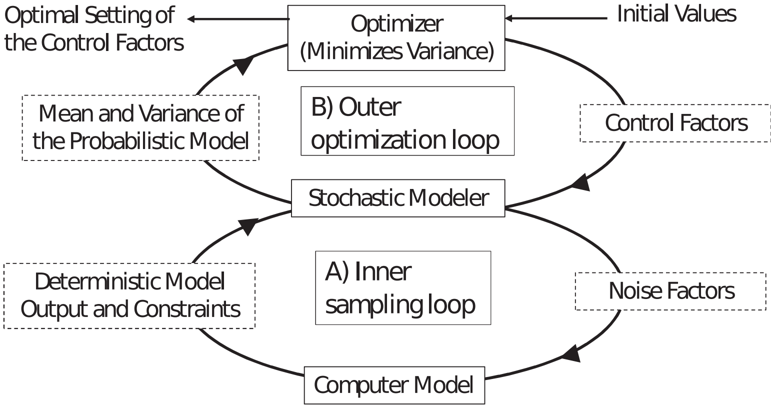

Figure 1. Schematic description of robust design including a sampling loop embedded within an optimization loop (Adapted from Kalagnanam & Diwekar 1997).

(Simpson *et al.* 2001). Therefore, it is generally acknowledged that the techniques for robust design via computer models ought to be different than the techniques for robust design via laboratory experiments. In response to this fact, the field of design and analysis of computer experiments (DACE) has grown rapidly in recent decades providing a variety of useful techniques (Santner *et al.* 2003). A review of the emerging field of DACE was provided by Giunta *et al.* (2003). Three of the most promising techniques developed so far are reviewed in the next paragraphs.

Robust design with computer experiments is often accomplished using a strategy employing two nested loops as depicted in Figure 1, an inner sampling loop and an outer optimization loop (Kalagnanam & Diwekar 1997; Du & Chen 2002; Lu & Darmofal 2005). The goal of robust design with computer experiments is to determine the optimal setting of control factors that minimizes the variance of the probabilistic model, while ensuring that the mean of the probabilistic model remains at the target value. The mean and variance are calculated by repeatedly running the deterministic computer model with different values of noise factors which are generated by a sampling scheme. Thus, the inner sampling loop comprises the probabilistic model and the outer optimization loop serves to decrease the variance of the probabilistic model's output.

2. Ways to implement the inner sampling loop

LHS is a stratified sampling technique that can be viewed as an extension of Latin square sampling and a close relative of highly fractionalized factorial designs (McKay *et al.* 1979). LHS ensures that each input variable has all portions of its distributions represented by input values. This is especially advantageous when only a few of the many inputs turn out to contribute significantly to the output variance. It has been proven that, for large samples, LHS provides smaller variance in estimators than simple random sampling as long as the response function is monotonic in all the noise factors (McKay *et al.* 1979). In typical engineering applications, LHS converges to 1% accuracy in estimating variance in about 2000 samples. However, there is also evidence that LHS provides no significant practical advantage over simple random sampling if the response function is highly non-linear (Giunta *et al.* 2003) so the number of samples required to converge to 1% will

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sometimes be much larger than 2000. Latin hypercube design continues to be an active area of improvement. Chen and Xiong (2017) proposed a means to nest these designs so that sequential construction is enabled and the restriction to multiples of the original design is relaxed. With similar objectives, Kong et al. (2018) proposed new sliced designs that accommodate arbitrary sizes for different slices and also derived their sampling properties.

An innovation called Hammersley sequence sampling (HSS) appears to provide significant advantages over LHS (Kalagnanam & Diwekar 1997). HSS employs a quasi-Monte Carlo sequence with low discrepancy and good space-filling properties. In applications to simple functions, it has been demonstrated that HSS converges to 1% accuracy faster than LHS by a factor of from 3 to 100. In an engineering application, HSS converged to 1% accuracy in about 150 samples.

A methodology based on the quadrature factorial model (QFM) employs fractional factorial designs augmented with a center point as a sampling scheme. A local regression model is formed based on these samples. This model is then used to generate the missing samples from a "contrived" full factorial 3^k design. Finally, this 3^k design is used to estimate the expected performance and deviation index. This method was shown to produce reasonable estimates with fewer samples especially for systems with significant interaction effects and nonlinear behavior (Yu & Ishii 1998).

Quadrature and cubature are techniques for exactly integrating specified classes of functions by means of a small number of highly structured samples. A remarkable number of different methods have been proposed for different regions and weighting functions (see Cools & Rabinowitz (1993) and Cools (1999), for reviews). More recently, Lu & Darmofal (2005) developed a cubature method for Gaussian weighted integration that scales better than other, previously published cubature schemes. If the number of uncertain factors in the inner loop is m, then the method requires $m^2 + 3m + 3$ samples. The new rule provides exact solutions for the mean for polynomials of fifth degree including the effects of all multifactor interactions. Used recursively to estimate transmitted variance, it provides exact solutions for polynomials of second degree including all two-factor interactions. On a challenging engineering application, the cubature method had less than 0.1% error in estimating mean and about 1% to 3% error in estimating variance. Quadratic scaling with dimensionality limits the method to applications with a relatively small number of uncertain factors.

A meta-model approach has been widely used in practice to overcome computational complexity (Booker *et al.* 1999; Simpson *et al.* 2001; Hoffman *et al.* 2003; Du *et al.* 2004). The term "meta-model" denotes a user-defined cheap-to-compute function which approximates the computationally expensive model. The popularity of the meta-model approach is due to (1) the cost of computer models of high fidelity in many engineering applications and (2) the many runs that are required for robust design, for which direct computing may be prohibitive. Although the meta-model approach has become a popular choice in many engineering designs, it does have some limitations. One difficulty associated with the meta-model approach is the challenge of constructing an accurate meta-model to represent the original model from a small sample size (Jin *et al.* 2000; Ye *et al.* 2000). These meta-model-based approaches continue to be improved and integrated with the optimization process (a departure from the nested loop structure displayed in Figure 1). For example, Iooss & Marrel (2019) combined several statistical tools

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including space-filling design, variable screening and Gaussian process metamodeling. The combined approach enabled consideration of a large number of variables and a more accurate estimation of confidence intervals for the results.

In meta-model-based approaches to robust design, acquisition functions are often used to sequentially determine the next design point so that a Gaussian Process emulator can more accurately locate the optimal setting. Tan (2020) proposed four new acquisition functions for optimizing expected quadratic loss, analyzed their convergence and developed accurate methods to compute them. Tan applied acquisition functions to robust parameter design problems with internal noise factors based on a Gaussian process model and an initial design tailored for such problems. On relatively simple functions, the proposed methods outperformed an optimization approach based on modeling the quadratic loss as a Gaussian Process and also performed better than maximin Latin hypercube designs. However, the proposed methods do not scale well to a large number of noise factors.

A method for robust parameter design using computer models was proposed by Tan & Wu (2012) using a Bayesian framework and Gaussian process metamodels. They proposed an expected quadratic loss criterion derived by taking expectation with respect to the noise factors and the posterior predictive process. An advantage of the approach is that it provides accurate Bayesian credible intervals for the average quadratic loss. This is valuable because the practitioner will benefit from not only a recommended set point for the control factors but also an interval estimate for the quality loss. These credible intervals are constructed via numerical inversion of the Lugannani–Rice saddlepoint approximation. A relationship between the quadrature method proposed here and the Tan and Wu approach is that integration required for computing the credible intervals used a three- or four-point quadrature method for evaluating the integral needed to find the cumulative density function for quadratic loss. An important difference is that Tan and Wu assumed that the distribution of the noise factors is discrete, or can be discretized. By contrast, the method proposed here assumes that the noise factors are normally distributed or else that they are adequately represented for the purpose of robust parameter design by their first two moments. Also, instead of confidence intervals on quadratic loss, our method provides an estimate of mean and variance of the error of its results.

Joseph *et al.* (2020) proposed a method for robust design with computer experiments with particular emphasis on nominal, discrete, and ordinal factors. The experimental designs are constructed to follow a maximum projection criterion which can simultaneously optimize the space-filling properties of the design points. This was an important development for instances when various types of factors are mixed in the problem domain because the optimal design criterion incorporating different types of input factors can produce much better experimental designs.

3. Motivation for this paper

The motivation for this paper is that LHS and HSS still require too many samples for many practical engineering applications. Computer models of adequate fidelity can require hours or days to execute. In some cases, changing input parameters to the computer models is not an automatic process – it can often require careful

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attention to ensure that the assumptions and methods of the analysis remain reasonable. It is also frequently the case that the results of computer models must be reviewed by experts or that some human intervention is required to achieve convergence. All of these considerations suggest a demand for techniques requiring a very small number of samples. Although QFM is designed to meet these needs, further improvements seem to be desirable.

Based on the considerations presented above, Frey *et al.* (2005) were motivated to develop a technique for computer experiments requiring a very small number of samples. They found that a five-point quadrature formula could be extended to multiple dimensions resulting in a $4d + 1$ formula that provided generally very good outcomes. Using case studies and a model-based evaluation, they showed that the quadrature technique can estimate the standard deviation within 5% in over 95% of systems which is far superior to LHS or HSS. Cubature performs somewhat better than quadrature with a similar number of samples given low dimensional problems, but cubature scales with the square of the dimension rather than linearly.

A concern regarding the quadrature-based technique is that its theoretical foundations were unclear. In particular, the extension to multiple dimensions seemed to be poorly justified. Therefore, the empirically demonstrated performance of the method presents a puzzle. This paper is the result of our efforts to establish a theoretical foundation and enable practitioners to better understand the assumptions required for its use.

4. Single variable Hermite–Gauss formula

As discussed in the introduction, robust parameter design requires a procedure to estimate the variance of the response of an engineering system in the presence of noise factors. Estimating the variance of a function involves computing an integral. One basic integration technique is Hermite–Gaussian quadrature. First, let us consider a one-dimensional case. Let us denote the response of the system as y and a single noise factor as z. If the noise factor is a standard normal variate, then the expected value of y can be estimated by a five-point Hermite–Gaussian quadrature formula. Figure 2 describes the concept as applied to an arbitrary function $y(z)$ and depicting the noise factor z as having zero mean to simplify the graphic.

The function is sampled at five points. One sample is at the mean of the variable z which is zero for this example. The other four samples are distributed symmetrically about the origin at prescribed points. The values of the function $y(z)$ are

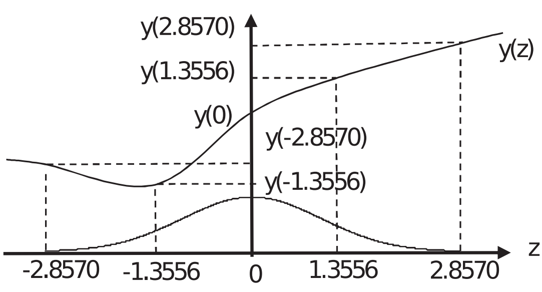

Figure 2. Five-point Hermite–Gauss Quadrature applied to an arbitrary function with the noise factor shifted and scaled to have zero mean and unit variance.

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weighted and summed to provide an estimate of the expected value. The sample points and weights in the following equation are selected so that the Hermite–Gaussian quadrature formula gives exact results if $y(z)$ is a polynomial of degree nine or less (Stroud & Seacrest 1966). The five-point Hermite–Gaussian quadrature formula is

$$\begin{gathered} Ey(z)) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}z^2} y(z) dz \approx \\ y(0) + \frac{1}{\sqrt{\pi}} \begin{bmatrix} A_1[y(\zeta_1) - y(0)] + A_1[y(-\zeta_1) - y(0)] + \\ A_2[y(\zeta_2) - y(0)] + A_2[y(-\zeta_2) - y(0)] \end{bmatrix}, \end{gathered} \tag{1}$$

with weights $A_1 = 0.39362\left(= \frac{1}{60}\left(7 + 2\sqrt{10}\right)\sqrt{\pi}\right)$, $A_2 = 0.019953\left(= \frac{1}{60}\left(7 - 2\sqrt{10}\right)\sqrt{\pi}\right)$ and sample points $\zeta_1 = 1.3556\left(= \sqrt{5 - \sqrt{10}}\right)$ and $\zeta_2 = 2.8570\left(= \sqrt{5 + \sqrt{10}}\right)$.

Estimating variance also involves computing an expected value, namely $E\left[(y(z) - E[y(z)])^2\right]$. By using Eq. (1) recursively, a variance estimate can be made using the same five samples although the approach gives exact results only if $y(z)$ is a polynomial of degree four or less.

$$\begin{aligned} E\left[(y(z) - E[y(z)])^2\right] &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}z^2} (y(z) - E[y(z)])^2 dz \\ &\approx [y(0) - E(y(z))]^2 + \\ &\frac{1}{\sqrt{\pi}} \begin{bmatrix} A_1\left[(y(\zeta_1) - E(y(z)))^2 - (y(0) - E(y(z)))^2\right] + \\ A_1\left[(y(\zeta_1) - E(y(z)))^2 - (y(0) - E(y(z)))^2\right] + \\ A_2\left[(y(\zeta_2) - E(y(z)))^2 - (y(0) - E(y(z)))^2\right] + \\ A_2\left[(y(-\zeta_2) - E(y(z)))^2 - (y(0) - E(y(z)))^2\right] \end{bmatrix} \\ &= \frac{1}{\sqrt{\pi}} \begin{bmatrix} A_1\left[(y(\zeta_1) - y(0))^2 + (y(-\zeta_1) - y(0))^2\right] + \\ A_2\left[(y(\zeta_2) - y(0))^2 + (y(-\zeta_2) - y(0))^2\right] \end{bmatrix} \\ &- \frac{1}{\sqrt{\pi}} \begin{bmatrix} A_1(y(\zeta_1) + y(-\zeta_1)) - 2(y(0)) + \\ A_2(y(\zeta_2) + y(-\zeta_2)) - 2(y(0)) \end{bmatrix}^2. \end{aligned} \tag{2}$$

5. Multiple variables Hermite–Gauss formula

In the multidimensional case, estimation of integrals becomes more complex. A variety of cubature formulae for Gaussian weighted m-dimensional integrals have been derived (Stroud 1971). These cubature techniques all scale poorly with the dimensionality of the integral despite recent improvements. For responses with more than about 10 variables, cubature will require too many samples to meet the stated goals.

To circumvent the problem of scaling in multidimensional integrals, it is proposed that a one-dimensional quadrature rule can be adapted to m-dimensional problems. The expected value of a function y is approximated by

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$$E(y(z)) \approx y(\bar{z}) + \sum_{i=1}^{m} \sum_{j=1}^{i-1} \alpha_i^{(j)} \left[y\left(\mathbf{D}_i^{(j)} e_i + \bar{z} \right) - y(\bar{z}) \right],$$

$$e_i = [\delta_{1i}\ \delta_{2i} \cdots\ \delta_{ni}] \text{ and } \delta_{ni} = \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{if } i = j, \end{cases} \tag{3}$$

The variance of the function y is approximated by

$$\sigma^2(y(z)) \approx \sum_{i=1}^{m} \left[\left(y(\bar{z}) + \sum_{j=1}^{i-1} \alpha_i^{(j)} \left[y\left(D_i^{(j)} + \bar{z} \right) - y(\bar{z}) \right] \right)^2 - \left[y^2(\bar{z}) + \sum_{i=1}^{m} \sum_{j=1}^{i-1} \alpha_i^{(j)} \left[y^2\left(D_i^{(j)} + \bar{z} \right) - y^2(\bar{z}) \right] \right] \right], \tag{4}$$

where $\mathbf{D}^{\langle i \rangle}$ denotes the ith row of the design matrix $\mathbf{D}$. For the quadrature-based method with $4m + 1$ samples and the design matrix $\mathbf{D}$ is

$$\mathbf{D} = \begin{bmatrix} +\zeta_1 \cdot \mathbf{I} \\ \hline -\zeta_1 \cdot \mathbf{I} \\ \hline +\zeta_2 \cdot \mathbf{I} \\ \hline -\zeta_2 \cdot \mathbf{I} \end{bmatrix}, \quad \mathbf{I} = \begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix}_{m \times m}. \tag{5}$$

This requires $4m + 1$ samples. The values of A_1 and A_2 and of ζ_1 and ζ_2 are the same as in the one-dimensional case.

A graphical depiction of the design for three standard normal variables ($m = 3$) and using $4m + 1$ samples is presented in Figure 3. The sampling scheme is composed of one center point and four axial runs per variable. Thus, the sampling pattern is similar to a star pattern in a central composite design.

6. Developing expressions for the method's error

The accuracy of the Hermite–Gaussian quadrature method in estimating the mean and variance can be verified using a Taylor series expansion.

In accordance with the previous sections, the accuracy of the Hermite–Gaussian quadrature method is first illustrated for a function of only one noise

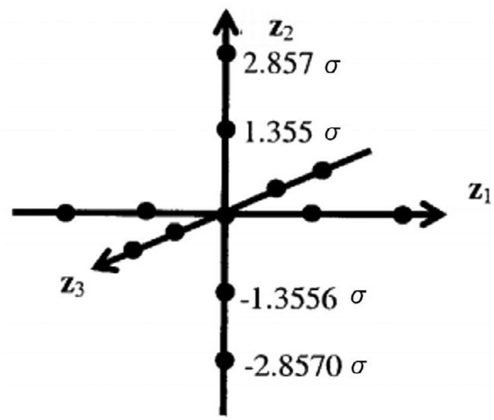

Figure 3. The sampling arrangement of the proposed quadrature-based method.

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factor following a standard normal distribution. If the response function $y(z)$ is continuous and differentiable, then the Taylor series approximation of $y(z)$ at $z=0$ is

$$y(z)=y(0)+y^{(1)}(0)z+\frac{y^{(2)}(0)}{2!}z^2+\frac{y^{(3)}(0)}{3!}z^3+\cdots. \tag{6}$$

For legibility reasons, from now on $\frac{y^{(i)}(0)}{i!}$, which is the polynomial coefficient of z^i, is replaced by $\beta^{(i)}$. With $z\tilde{}\ N(0,1)$, if the coefficients were known, the exact expected value of $y(z)$ could be calculated as

$$\begin{aligned}E[y(z)]&=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{-\frac{1}{2}z^2}\sum_{n=0}^{\infty}\beta^{(n)}z^n dz\\&=\frac{1}{\sqrt{2\pi}}\sum_{n=0}^{\infty}\beta^{(n)}\int_{-\infty}^{\infty}e^{-\frac{1}{2}z^2}z^n dz\\&=\frac{1}{\sqrt{2\pi}}\sum_{k=0}^{\infty}\beta^{(2k)}\int_{-\infty}^{\infty}e^{-\frac{1}{2}z^2}z^{2k}dz\\&=\sum_{k=0}^{\infty}\frac{(2k)!}{2^k k!}\beta^{(2k)}.\end{aligned} \tag{7}$$

In contrast, the expected value of $y(z)$ can also be estimated using the quadrature-based method, again using the Taylor series of $y(z)$,

$$\begin{aligned}E(y(z))&=\int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}}e^{-\frac{1}{2}z^2}y(z)dz\\&\approx y(0)+\frac{1}{\sqrt{\pi}}\begin{bmatrix}A_1[y(\zeta_1)-y(0)]+A_1[y(-\zeta_1)-y(0)]+\\A_2[y(\zeta_2)-y(0)]+A_2[y(-\zeta_2)-y(0)]\end{bmatrix}\\&=y(0)+\frac{2}{\sqrt{\pi}}\left[\sum_{k=1}^{\infty}\beta^{(2k)}\left[A_1\zeta_1^{2k}+A_2\zeta_2^{2k}\right]\right].\end{aligned} \tag{8}$$

Elaboration of Eq. (7) yields

$$\begin{aligned}E[y(z)]_{\text{exact}}=&\beta^{(0)}+\beta^{(2)}+3\beta^{(4)}+15\beta^{(6)}+\\&105\beta^{(8)}+945\beta^{(10)}+10395\beta^{(12)}+\cdots.\end{aligned} \tag{9}$$

Elaboration of Eq. (8) yields

$$\begin{aligned}E[y(z)]_{\text{quadr}}=&\beta^{(0)}+\beta^{(2)}+3\beta^{(4)}+15\beta^{(6)}+\\&105\beta^{(8)}+825\beta^{(10)}+6675\beta^{(12)}+\cdots.\end{aligned} \tag{10}$$

The coefficients of the first five terms are equal. Therefore, for polynomials of degree less than 9 the quadrature method will give exact solutions.

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Substituting the Taylor series approximation of $y(z)$ at $z = 0$ allows the exact value of variance of $y(z)$ to be expressed as a function of the coefficients:

$$\begin{aligned}\mathrm{var}(y(z)) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2}z^2} y^2(z)dz - \left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2}z^2} y(z)dz\right]^2 \\ &= \sum_{k=0}^{\infty}\frac{(2k)!}{2^k k!}\sum_{i=0}^{2k}\beta^{(i)}\beta^{(2k-i)} - \left[\sum_{k=0}^{\infty}\frac{(2k)!}{2^k k!}\beta^{(2k)}\right]^2,\end{aligned} \tag{11}$$

The variance of $y(z)$ can also be estimated using the quadrature-based method,

$$\begin{aligned}\mathrm{var}(y(z)) &\approx \frac{1}{\sqrt{\pi}}\begin{bmatrix} A_1\left[(y(\zeta_1)-y(0))^2+(y(-\zeta_1)-y(0))^2\right]+ \\ A_2\left[(y(\zeta_2)-y(0))^2+(y(-\zeta_2)-y(0))^2\right]\end{bmatrix} \\ &\quad -\frac{1}{\pi}\begin{bmatrix} A_1(y(\zeta_1)+y(-\zeta_1)-2y(0))+ \\ A_2(y(\zeta_2)+y(-\zeta_2)-2y(0))\end{bmatrix}^2 \\ &= \frac{2}{\sqrt{\pi}}\left[\sum_{k=1}^{\infty}\left(\sum_{j=1}^{2k-1}\beta^{(j)}\beta^{(2k-j)}\right)\left[A_1\zeta_1^{2k}+A_2\zeta_2^{2k}\right]\right] \\ &\quad -\frac{4}{\pi}\left[\sum_{k=1}^{\infty}\beta^{(2k)}\left[A_1\zeta_1^{2k}+A_2\zeta_2^{2k}\right]\right]^2.\end{aligned} \tag{12}$$

Elaboration of Eq. (11) yields

$$\begin{aligned}\mathrm{var}(y(z))_{\mathrm{exact}} = {}& \left(\beta^{(1)}\right)^2 + \left(6\beta^{(1)}\beta^{(3)} + 2\left(\beta^{(2)}\right)^2\right) + \left(30\beta^{(1)}\beta^{(5)} + 24\beta^{(2)}\beta^{(4)} + 15\left(\beta^{(3)}\right)^2\right) + \\ & \left(210\beta^{(1)}\beta^{(7)} + 180\beta^{(2)}\beta^{(6)} + 210\beta^{(3)}\beta^{(5)} + 96\left(\beta^{(4)}\right)^2\right) + \\ & \left(1890\beta^{(1)}\beta^{(9)} + 1680\beta^{(2)}\beta^{(8)} + 1890\beta^{(3)}\beta^{(7)} + 1800\beta^{(4)}\beta^{(6)} + 945\left(\beta^{(5)}\right)^2\right) + \cdots.\end{aligned}$$

Elaboration of Eq. (12) yields

$$\begin{aligned}\mathrm{var}(y(z))_{\mathrm{exact}} = {}& \left(\beta^{(1)}\right)^2 + \left(6\beta^{(1)}\beta^{(3)} + 2\left(\beta^{(2)}\right)^2\right) + \left(30\beta^{(1)}\beta^{(5)} + 24\beta^{(2)}\beta^{(4)} + 15\left(\beta^{(3)}\right)^2\right) + \\ & \left(210\beta^{(1)}\beta^{(7)} + 180\beta^{(2)}\beta^{(6)} + 210\beta^{(3)}\beta^{(5)} + 96\left(\beta^{(4)}\right)^2\right) + \\ & \left(1650\beta^{(1)}\beta^{(9)} + 1440\beta^{(2)}\beta^{(8)} + 1650\beta^{(3)}\beta^{(7)} + 1560\beta^{(4)}\beta^{(6)} + 825\left(\beta^{(5)}\right)^2\right) + \cdots.\end{aligned}$$

The coefficients of the first 10 terms are equal. Therefore, for polynomials of degree less than 5, the quadrature method will give exact solutions for the variance.

Now consider the case for m random input variables, all independent and following a standard normal distribution (without loss of generality because scaling and shifting of the variable z is accomplished relatively simply). Assuming the function is separable, $y(z)$ can be written as $\sum_{j=1}^{m} y_j(z_j)$.

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To simplify notation, from this point forward, $\frac{1}{i!}\frac{\partial^i y}{\partial z_j^i}(\underline{0})$, which is the polynomial coefficient of z_j^i, is replaced by $\beta_j^{(i)}$.

In that case, the Taylor series approximation of $y(z)$ around $z = (0, 0, \ldots, 0)$ is

$$y(z) = y(0) + \sum_{n=1}^{\infty}\sum_{j=1}^{m}\left[\beta_j^{(n)} z_j^n\right]. \tag{13}$$

And corresponding with Eq. (7) the expected value of $y(z)$ equals

$$E[y(z)] = y(0) + \sum_{k=1}^{\infty}\frac{(2k)!}{2^k k!}\sum_{j=1}^{m}\beta_j^{(2k)}. \tag{14}$$

Using the quadrature-based method, the expected value of $y(z)$ can also be estimated,

$$\begin{aligned} E(y(\underline{z})) &= \sum_{j=1}^{m} E\left(y_j(z_j)\right) \\ &\approx y(\underline{0}) + \frac{2}{\sqrt{\pi}}\sum_{j=1}^{m}\left[\sum_{k=1}^{\infty}\left[A_1\zeta_1^{2k} + A_2\zeta_2^{2k}\right]\beta_j^{(2k)}\right]. \end{aligned} \tag{15}$$

Elaboration of both Eqs. (14) and (15) gives a similar result as in the one-dimensional case. For continuous, differentiable and separable polynomials of degree less than 10 the quadrature method will give exact solutions for the expected value.

The relative error mean is obtained by subtracting Eq. (15) from Eq. (14) and then dividing by Eq. (14).

$$\text{Rel\_error} = \frac{-\sum_{j=1}^{m}\left[120\beta_j^{(10)} + 3720\beta_j^{(12)} + \ldots\right]}{y(\overline{z}) + \sum_{j=1}^{m}\left[\beta_j^{(2)} + 3\beta_j^{(4)} + 15\beta_j^{(6)} + 105\beta_j^{(8)} + 945\beta_j^{(10)} + 10395\beta_j^{(12)} + \ldots\right]}. \tag{16}$$

The coefficients in the numerator are typically very small. And it is also likely that the term $y(\overline{z})$ in the denominator is the dominating term in practical engineering systems. Hence the quadrature-based method gives accurate results in estimating the expected value for 10th or higher order separable polynomial systems.

Corresponding with Eq. (11), the variance of $y(z)$ equals

$$\text{var}(y(z)) = \sum_{j=1}^{m}\left[\sum_{k=0}^{\infty}\frac{(2k)!}{2^k k!}\sum_{i=0}^{2k}\beta_j^{(i)}\beta_j^{(2k-i)} - \left[\sum_{k=0}^{\infty}\frac{(2k)!}{2^k k!}\beta_j^{(2k)}\right]^2\right]. \tag{17}$$

Using the quadrature-based method, the variance of $y(z)$ can also be estimated

$$\text{var}(y(z)) \approx \left[\sum_{j=1}^{m}\begin{array}{l}\frac{2}{\sqrt{\pi}}\left[\sum_{k=1}^{\infty}\left(\sum_{i=1}^{2k-1}\beta_j^{(i)}\beta_j^{(2k-i)}\right)\left[A_1\zeta_1^{2k} + A_2\zeta_2^{2k}\right]\right] \\ -\frac{4}{\pi}\left[\sum_{k=1}^{\infty}\beta_j^{(2k)}\left[A_1\zeta_1^{2k} + A_2\zeta_2^{2k}\right]\right]^2\end{array}\right]. \tag{18}$$

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The relative error mean is obtained by subtracting Eq. (18) from Eq. (17) and then divided by Eq. (17)

$$\varepsilon_{\sigma^2}=\sum_{j=1}^{m}\frac{-240\left(\beta_j^{(1)}\beta_j^{(9)}+\beta_j^{(2)}\beta_j^{(8)}+\beta_j^{(3)}\beta_j^{(7)}+\beta_j^{(4)}\beta_j^{(6)}+\frac{1}{2}\left(\beta_j^{(5)}\right)^2\right)-\cdots}{\left(\beta_j^{(1)}\right)^2+\left(6\beta_j^{(1)}\beta_j^{(3)}+2\left(\beta_j^{(2)}\right)^2\right)+\left(30\beta_j^{(1)}\beta_j^{(5)}+24\beta_j^{(2)}\beta_j^{(4)}+15\left(\beta_j^{(3)}\right)^2\right)+\cdots}. \tag{19}$$

The coefficients in the numerator are again small. Hence the quadrature-based method gives accurate results in estimating the variance for 5th or higher order separable polynomial systems.

7. Statistical properties of error

For the following results, we assume continuous, differentiable and separable polynomials with polynomial coefficients that are mutually independent and normally distributed with zero mean and variances that decrease geometrically at rate r with the increasing of polynomial order, that is, $\beta_j^{(i)}\sim N(0,r^i)$.

For polynomials satisfying these properties, we can derive exact formulas for the expected value and the variance of the error ε_{σ^2} in Eq. (19). Essential to this effort is a theorem proved by Magnus (1986), which will be presented in its entirety here.

Theorem 1 (Magnus 1986)

Let x be a normally distributed $n\times 1$ vector with mean μ and positive definite covariance matrix $\Omega=LL^T$. Let A be a symmetric $n\times n$ matrix and B a positive semidefinite $n\times n$ matrix, $B\neq 0$. Let P be an orthogonal $n\times n$ matrix and Λ a diagonal $n\times n$ matrix such that

$$P^TL^TBLP=\Lambda,\quad P^TP=I_n$$

and define

$$A^*=P^TL^TALP,\quad \mu^*=P^TL^{-1}\mu.$$

Then we have, provided the expectation exists, for $s=1,2,\ldots$

$$E\left[\frac{x^TAx}{x^TBx}\right]^s=\frac{e^{-\frac{1}{2}\mu^T\Omega^{-1}\mu}}{(s-1)!}\sum_{v}\gamma_s(v)\times\int_0^\infty t^{s-1}|\Delta|e^{\frac{1}{2}\xi^T\xi}\prod_{j=1}^{s}\left(trR^j+j\xi^TR^j\xi\right)^{n_j}dt,$$

where the summation is over all $1\times s$ vectors $v=(n_1,n_2,\ldots,n_s)$ whose elements n_j are nonnegative integers satisfying $\sum_{j=1}^{s}jn_j=s$,

$$\gamma_s(v)=s!2^s\prod_{j=1}^{s}\left[n_j!(2j)^{n_j}\right]^{-1}$$

and Δ is a diagonal positive definite $n\times n$ matrix, R a symmetric $n\times n$ matrix and x an $n\times 1$ vector given by

$$\Delta=(I_n+2t\Lambda)^{-\frac{1}{2}},\quad R=\Delta A^*\Delta,\quad \xi=\Delta\mu^*.$$

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Let $y(z_1, z_2, \ldots, z_m)$ be a continuous, differentiable, separable polynomial of order n. Let x_j be the vector of normally distributed polynomial coefficients of the variable z_j in increasing order, that is, $x_j = \left(\beta_j^{(1)}, \beta_j^{(2)}, \ldots, \beta_j^{(n)}\right)$. In that case, its mean $\mu = 0$, $\xi = \Delta\mu^* = 0$ and the covariance matrix Ω is a diagonal matrix with $[r, r^2, \ldots, r^n]$ on its diagonal.

Let A be the $n \times n$ matrix with $A_{i_1,i_2}, i_1 \neq i_2$, is half the coefficient of $\beta_j^{(i_1)}\beta_j^{(i_2)}$ and $A_{i,i}$ is the coefficient of $\left(\beta_j^{(i)}\right)^2$ in the numerator of Eq. (19). Let B be the $n \times n$ matrix with $B_{i_1,i_2}, i_1 \neq i_2$, is half the coefficient of $\beta_j^{(i_1)}\beta_j^{(i_2)}$ and $B_{i,i}$ is the coefficient of $\left(\beta_j^{(i)}\right)^2$ in the denominator of Eq. (19). Then

$\varepsilon_{\sigma^2} = \frac{x^T A x}{x^T B x}$ and we can apply Theorem 1 for $s = 1$, giving the expected value and for $s = 2$, giving the variance of ε_{σ^2}.

Theorem 2

Let $y(z_1, z_2, \ldots, z_m)$ be a continuous, differentiable, separable polynomial of order n with polynomial coefficients that are mutually independent and normally distributed with zero mean and variances that decrease geometrically at rate r with the increasing of polynomial order, that is, $\beta_j^{(i)} \sim N(0, r^i)$.

Then the relative error ε_{σ^2} of the quadrature method has mean

$$\mathrm{E}[\varepsilon_{\sigma^2}] = m \int_0^\infty \left(\prod_{i=1}^n \frac{1}{\sqrt{1+2t\lambda_i}}\right)^m \left(\sum_{i=1}^n \frac{1}{(1+2t\lambda_i)} \sum_{k=1}^n \sum_{l=1}^n \sqrt{r^{k+l}} P_{k,i} P_{l,i} A_{k,l}\right) dt$$

and variance

$$\mathrm{E}[\varepsilon_{\sigma^2}]^2 = m \int_0^\infty \left(\prod_{i=1}^n \frac{t}{\sqrt{1+2t\lambda_i}}\right)^m \sum_{i_1=1}^n \sum_{i_2=1}^n \frac{X_{i_1 i_2}}{(1+2t\lambda_{i_1})(1+2t\lambda_{i_2})} dt$$

with

$$X_{i_1 i_2} = \sum_{k_1=1}^n \sum_{k_2=2}^n \sum_{l_1=1}^n \sum_{l_2=1}^n \sqrt{r^{k_1+k_2+l_1+l_2}} P_{i_1,l_1} P_{i_2,l_2} (2P_{i_2,k_1} P_{i_1,k_2} + P_{i_1,k_1} P_{i_2,k_2}) A_{l_1,k_1} A_{l_2,k_2}.$$

Here λ is a vector of eigenvalues and P is a matrix whose columns correspond to the eigenvectors of the matrix $M = L^T B L$, with B the $n \times n$ matrix with $B_{i_1,i_2}, i_1 \neq i_2$, is half the coefficient of $\beta_j^{(i_1)}\beta_j^{(i_2)}$ and $B_{i,i}$ is the coefficient of $\left(\beta_j^{(i)}\right)^2$ in the denominator of Eq. (19) and L is a diagonal matrix with $\left[\sqrt{r}, \sqrt{r^2}, \ldots, \sqrt{r^n}\right]$ on its diagonal.

Proof

For $s = 1$, we have $v = [1]$ and $\gamma_1([1]) = 1$.

For $s = 2$, we have $n_1 + 2n_2 = 2$, that is, $v = [0, 1]$ or $v = [2, 0]$, and $\gamma_2([0, 1]) = 2$ and $\gamma_2([2, 0]) = 1$.

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Let L be the diagonal matrix with $\left[\sqrt{r}, \sqrt{r^2}, \ldots, \sqrt{r^n}\right]$ on its diagonal, then $\Omega = LL^T$ and let

$$M = L^T BL.$$

Let P be an $n \times n$ matrix with the normalized eigenvectors of the matrix M as its columns, then $P^T P = I_n$ and

$$\Lambda = P^T L^T BLP$$

is the $n \times n$ diagonal matrix with the eigenvalues $\lambda_1, \ldots, \lambda_n$ of M on its diagonal. Let Δ be defined by

$$\Delta = (I_n + 2t\Lambda)^{-\frac{1}{2}} = \begin{bmatrix} \sqrt{1+2t\lambda_1} & 0 & 0 & \cdots & 0 \\ 0 & \sqrt{1+2t\lambda_2} & 0 & \cdots & 0 \\ 0 & 0 & \sqrt{1+2t\lambda_3} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \sqrt{1+2t\lambda_n} \end{bmatrix}^{-1}.$$

Then its determinant equals $|\Delta| = \prod_{i=1}^{n} \frac{1}{\sqrt{1+2t\lambda_i}}$.

Let A^* be defined by

$$A^* = P^T L^T ALP$$

Then $R = \Delta\, A^*\, \Delta$ equals

$$R = (I_n + 2t\Lambda)^{-1/2} P^T L^T ALP (I_n + 2t\Lambda)^{-1/2}.$$

The elements of R equal

$$R_{i_1,i_2} = \frac{1}{\sqrt{(1+2t\lambda_{i_1})(1+2t\lambda_{i_2})}} \sum_{k=1}^{n} \sum_{l=1}^{n} \sqrt{r^{k+l}} P_{i_1,k} P_{i_2,l} A_{l,k}, i_1, i_2 \in \{1, 2, \ldots, n\}.$$

The diagonal elements of R^2 equal

$$R^2_{i_1,i_1} = \sum_{i_2=1}^{n} R_{i_2 i_1} R_{i_1 i_2}, i_1 \in \{1, 2, \ldots, n\}.$$

Then

$$\mathrm{E}[\varepsilon_{\sigma^2}] = \sum_{j=1}^{m} \int_0^\infty |\Delta| \operatorname{tr} R dt$$

$$= m \int_0^\infty \left(\prod_{i=1}^{n} \frac{1}{\sqrt{1+2t\lambda_i}} \right)^m \left(\sum_{i=1}^{n} \frac{1}{(1+2t\lambda_i)} \sum_{k=1}^{n} \sum_{l=1}^{n} \sqrt{r^{k+l}} P_{k,i} P_{l,i} A_{k,l} \right) dt$$

and

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$$\begin{aligned}
\mathrm{E}[\varepsilon_{\sigma^2}]^2 &= \sum_{j=1}^{m} 2\int_0^\infty t|\Delta|\left(\operatorname{tr} R^2\right)dt + \int_0^\infty t|\Delta|\left(\operatorname{tr} R\right)^2 dt \\
&= \sum_{j=1}^{m} \int_0^\infty t|\Delta|\left(2\operatorname{tr} R^2 + (\operatorname{tr} R)^2\right)dt \\
&= m\int_0^\infty \left(\prod_{i=1}^{n} \frac{t}{\sqrt{1+2t\lambda_i}}\right)^m \left(2\sum_{i_1=1}^{n}\sum_{i_2=1}^{n} R_{i_2 i_1} R_{i_1 i_2} + \left(\sum_{i_1=1}^{n} R_{i_1 i_1}\right)^2\right)dt \\
&= m\int_0^\infty \left(\prod_{i=1}^{n} \frac{t}{\sqrt{1+2t\lambda_i}}\right)^m \sum_{i_1=1}^{n}\sum_{i_2=1}^{n} (2R_{i_2 i_1} R_{i_1 i_2} + R_{i_1 i_1} R_{i_2 i_2})dt \\
&= m\int_0^\infty \left(\prod_{i=1}^{n} \frac{t}{\sqrt{1+2t\lambda_i}}\right)^m \sum_{i_1=1}^{n}\sum_{i_2=1}^{n} \frac{X_{i_1 i_2}}{(1+2t\lambda_{i_1})(1+2t\lambda_{i_2})}dt,
\end{aligned}$$

with

$$X_{i_1 i_2} = \sum_{k_1=1}^{n}\sum_{k_2=2}^{n}\sum_{l_1=1}^{n}\sum_{l_2=1}^{n} \sqrt{r^{k_1+k_2+l_1+l_2}} P_{i_1,l_1} P_{i_2,l_2} (2P_{i_2,k_1} P_{i_1,k_2} + P_{i_1,k_1} P_{i_2,k_2}) A_{l_1,k_1} A_{l_2,k_2}.$$

Assume that the function $y(\mathrm{z})$ is a fifth-order separable polynomial and that the polynomial coefficients are normally distributed with zero mean and their variance that decreases geometrically at rate r with the increasing of polynomial order. For a fifth order polynomial, the numerator of Eq. (19) only consists of the term $120\left(\beta_j^{(5)}\right)^2$, so $A_{5,5} = 120$ and $A_{i,j} = 0$ otherwise. Then, with Theorem 2, the relative error ε_{σ^2} of the quadrature method has mean

$$\mathrm{E}[\varepsilon_{\sigma^2}] = -120 r^5 m \int_0^\infty \left(\prod_{i=1}^{5} \frac{1}{\sqrt{1+2t\lambda_i}}\right)^m \left(\sum_{i=1}^{5} \frac{P_{5,i}^2}{(1+2t\lambda_i)}\right)dt$$

and variance

$$\mathrm{E}[\varepsilon_{\sigma^2}]^2 = 120^2 r^{10} m \int_0^\infty \left(\prod_{i=1}^{n} \frac{t}{\sqrt{1+2t\lambda_i}}\right)^m \sum_{i_1=1}^{n}\sum_{i_2=1}^{n} \frac{P_{i_1,5} P_{i_2,5}\left(2P_{i_2,5} P_{i_1,5} + P_{i_1,5} P_{i_2,5}\right)}{\left(1+2t\lambda_{i_1}\right)\left(1+2t\lambda_{i_2}\right)}dt.$$

An interesting implication of Theorem 2 is that the expected value of error is nonzero for polynomials of order 5 and higher and therefore the quadrature-based method is biased in estimating the relative error ε_{σ^2} for a fifth or higher order separable polynomial system.

Figure 4 presents results from Theorem 2 which can be used as *a priori* error estimates. Plotted are the expected value of error and the standard deviation of error for the quadrature-based method versus dimensionality m for a few different values of the parameter r. The plotted values were computed using Theorem 2 and confirmed via Monte Carlo simulation. The results are plotted over a range of values for the parameter r. It was shown empirically by Li & Frey (2005) via a meta-analysis of published experiments that two-factor interactions are about 0.2 the size of the main effects on average across large populations of factorial experiments. This might suggest that 0.2 is a reasonable mean value for a prior probability of r, but we also plotted results for somewhat higher and lower values of r.

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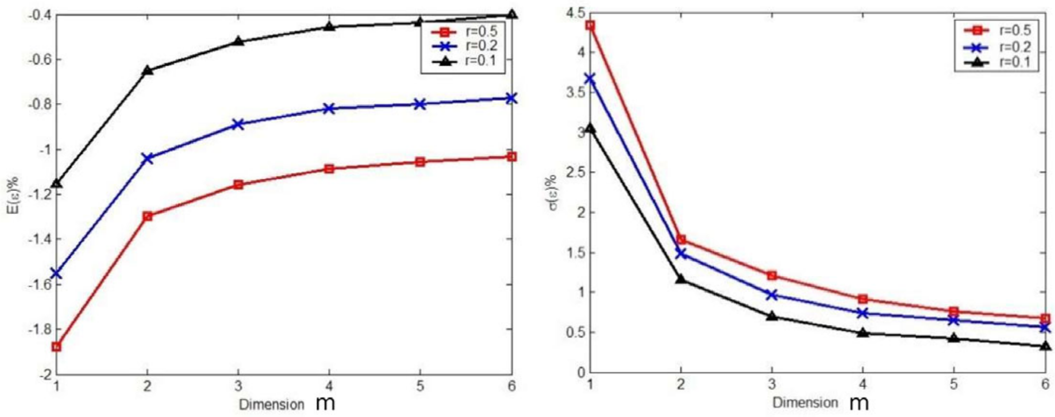

Figure 4. The scaling with dimensionality, m, of standard deviation of relative error, ε, for of the quadrature-based method when applied to separable functions.

The expected value of error for quadrature is strictly negative; therefore the estimates tend to be lower than the actual transmitted variance of the system, although the error can be positive in individual uses of the method. The mean error decreases and the dimensionality of the problem increases, but it does not converge asymptotically toward zero.

The first term in Eq. (17) is weighted by m while the second term is weighted by m^2 and the denominators of both terms are raised to the power m. An interesting implication is that, if the function y is separable, the error variance of the method decreases monotonically and tends to zero in the limit as the number of noise factors, m, grows. This monotonicity and decay to zero hold for all values of the rate of decay r less than unity.

8. Comparative assessment via hierarchical probability models

The accuracy of the proposed method is determined by the relative size of single-factor effects and interactions and by the number of interactions. Thus, an error estimate might be based on a reasonable model of the size and probability of interactions. The hierarchical probability model was proposed by Chipman *et al.* (1997) as a means to more effectively derive response models from experiments with complex aliasing patterns. This model was fit to data from 46 full factorial engineering experiments (Li and Frey, 2005). The fitted model is useful for evaluating various techniques for robust design with computer experiments. Eqs. (20) through (27) comprise the model used here.

$$y=\sum_{i=1}^{n}\beta_i x_i+\sum_{j=1}^{n}\sum_{\substack{i=1\\ i\le j}}^{n}\beta_{ij}x_i x_j+\sum_{k=1}^{n}\sum_{\substack{j=1\\ j\le k}}^{n}\sum_{\substack{i=1\\ i\le j}}^{n}\beta_{ijk}x_i x_j x_k \tag{20}$$

$$x_i\sim N\left(0,\sigma^2\right), \tag{21}$$

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where σ = 10%.

$$f(\beta_i|\delta_i) = \begin{cases} N(0,1) \text{ if } \delta_\mathrm{i} = 0 \\ N(0,10) \text{ if } \delta_\mathrm{i} = 1 \end{cases} \tag{22}$$

$$f\left(\beta_{ij}|\delta_{ij}\right) = \begin{cases} N(0,1) \text{ if } \delta_\mathrm{ij} = 0 \\ N(0,10) \text{ if } \delta_\mathrm{ij} = 1 \end{cases} \tag{23}$$

$$f\left(\beta_{ijk}|\delta_{ijk}\right) = \begin{cases} N(0,1) \text{ if } \delta_{ijk} = 0 \\ N(0,10) \text{ if } \delta_{ijk} = 1 \end{cases} \tag{24}$$

$$\Pr(\delta_i = 1) = p \tag{25}$$

$$\Pr\left(\delta_{ij} = 1|\delta_i,\delta_j\right) = \begin{cases} p_{00} \text{ if } \delta_\mathrm{i} + \delta_\mathrm{j} = 0 \\ p_{01} \text{ if } \delta_\mathrm{i} + \delta_\mathrm{j} = 1 \\ p_{11} \text{ if } \delta_\mathrm{i} + \delta_\mathrm{j} = 2 \end{cases} \tag{26}$$

$$\Pr\left(\delta_{ijk} = 1|\delta_i,\delta_j,\delta_k\right) = \begin{cases} p_{000} \text{ if } \delta_\mathrm{i} + \delta_\mathrm{j} + \delta_\mathrm{k} = 0 \\ p_{001} \text{ if } \delta_\mathrm{i} + \delta_\mathrm{j} + \delta_\mathrm{k} = 1 \\ p_{011} \text{ if } \delta_\mathrm{i} + \delta_\mathrm{j} + \delta_\mathrm{k} = 2 \\ p_{111} \text{ if } \delta_\mathrm{i} + \delta_\mathrm{j} + \delta_\mathrm{k} = 3 \end{cases} \tag{27}$$

Eq. (20) expresses the assumption that the system response is a third order polynomial. Eq. (21) defines the input variations as random normal variates. We used a standard deviation of 10% because it represented a level of difficulty for the methods comparable to that found in most case studies we have found in the literature. Eqs. (22) through (24) assign probability distributions to the polynomial coefficients. Polynomial coefficients $\beta_\imath$ whose corresponding parameter $\delta_\imath = 1$ have a larger probability of taking on a large positive or negative value. The values of the parameters $\delta_\imath$ are set in Eqs. (25) through (27). The values of the parameters in the model are taken from an empirical study of 113 full factorial experiments [16] and are $p = 39\%$, $p_{00} = 0.48\%$, $p_{01} = 4.5\%$, $p_{11} = 33\%$, $p_{000} = 1.2\%$, $p_{001} = 3.5\%$, $p_{011} = 6.7\%$ and $p_{111} = 15\%$.

For each integer $n \in [6, 20]$, one thousand systems were sampled from the model (Eqs. (20 through (27)) The expected value and standard deviation of the response y was estimated in five ways:

(i) using the quadrature technique which required $4m+1$ samples,
(ii) generating $4m+1$ samples via LHS and computing their mean and standard deviation,
(iii) generating $4m+1$ samples via HSS and computing their mean and standard deviation,
(iv) generating $10 \times (4m+1)$ samples via LHS and computing their mean and standard deviation and
(v) generating $10 \times (4m+1)$ samples via HSS and computing their mean and standard deviation.

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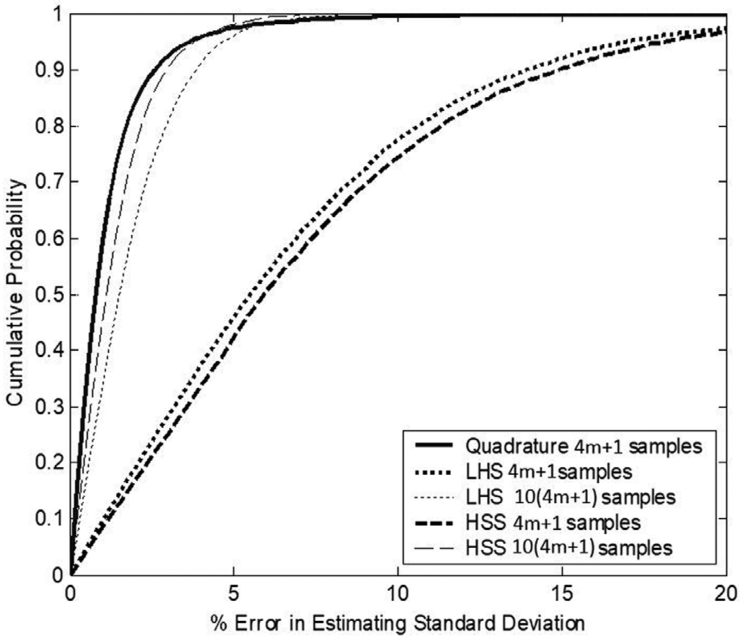

Figure 5. Cumulative probability versus error in estimating standard deviation for five different sampling procedures.

The exact solution was also determined using Eqs. (9 and (10), enabling the computation of the size of the error for each of the 1000 systems given each of the three methods. These data were used to estimate the cumulative probability versus error (Figure 4). In effect, this is a chart of confidence level versus error tolerance. The preference is for methods that lie higher on the chart since this indicates greater confidence that the given error tolerance will be satisfied than methods lower on the chart.

Figure 5 shows that the quadrature technique estimated the standard deviation within 5% for more than 95% of all systems sampled. Quadrature accomplished this with only $4m+1$ samples. HSS and LHS were unable to provide comparably good results with $4m+1$ samples. However, given 10 times the resources, HSS achieved accuracy comparable to that of quadrature.

The model-based evaluation presented here assumes that the system response is a polynomial. This is a significant limitation. This approach can reveal the error due to the presence of interaction effects, but it cannot account for the errors due to departure of a system from a polynomial response approximation. For this reason, the case studies in the next section are an important additional check on the results.

9. Comparative assessment via case studies

This section presents five computer simulations of engineering systems to which different methods for estimating transmitted variance are applied. One of the engineering systems, the LifeSat satellite, has two different responses making six responses total in the set of five systems. For each of the six responses, two designs within the parameter space are considered – an initial design and an alternative

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that exhibits lower transmitted variance (we will call this the “robust design”). As a result, there were 12 cases in total to which the sampling methods were applied.

9.1. Case 1: continuous-stirred tank reactor

The engineering system in this case is a continuous-stirred tank reactor (CSTR) which was used to demonstrate the advantages of HSS over LHS (McKay *et al.* 1979). The function of the CSTR system is to produce a chemical species B at a target production rate (R_B) of 60 mol/min. Variations from the target (either above or below target) are undesirable. The CSTR system is comprised of a tank into which liquid flows at a volumetric flow rate (F) and initial temperature (T_i). The liquid contains two chemical species (A and B) with known initial concentrations (C_{Ai} and C_{Bi}). In addition to fluid, heat is added to the CSTR at a given rate (Q). Fluid flows from the CSTR at the same rate it enters but at different temperature (T) and with different concentrations of the species A and B (C_A and C_B). The system is governed by five equations.

$$Q = F\rho C_p(T - T_i) + V(r_A H_{RA} + r_B H_{RB}),$$

$$C_A = \frac{C_{Ai}}{1 + k_A^0 e^{-E_A/RT}\tau},$$

$$C_B = \frac{C_{Bi} + k_A^0 e^{-E_A/RT}\tau C_A}{1 + k_B^0 e^{-E_B/RT}\tau},$$

$$-r_A = k_A^0 e^{-E_A/RT} C_A,$$

$$-r_B = k_B^0 e^{-E_B/RT} C_B - k_A^0 e^{-E_A/RT} C_A,$$

where the average residence time in the reactor is V/F and the realized production rate (R_B) is $r_B V$ which has a desired target of 60 mol/min.

Table 1 provides a listing of physical constants, input and output variables. These values of physical constants and the input variables are taken directly from Kalagnanam & Diwekar (1997)) with the exception that the values of T and T_i were swapped to correct for a typographical error in the previous paper pointed out to us by its authors. Following the example of Kalagnam and Diwekar’s paper, we assume that all the input variables are independent and normally distributed with a standard deviation of 10% of the mean. We considered two different “designs” (i.e., nominal values for the input variables) described in Kalagnam and Diwekar’s paper – one was an initial design and the other was an optimized robust design with greatly reduced variance in the response R_B.

To check that the model was correctly implemented, the results at both points were reproduced by Monte Carlo simulations with 10^6 trials each. Kalagnam and Diwekar found a transmitted variance in the initial design of 1638 (mol/min)^2 and we computed a transmitted variance of 1625.7 $\pm$ 1.5 (mol/min)^2. There was also a small discrepancy in the transmitted variance of the robust design – the published value was 232 (mol/min)^2 and we computed 232.3 $\pm$ 0.4 (mol/min)^2. The

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Table 1. Parameters and their values in the continuous-stirred tank reactor case study

Parameter	Value	Units	Description
k_A^0	8.4 x 10^5	1/min	Constant
k_B^0	7.6 x 10^4	1/min	Constant
H_{RA}	−2.12 x 10^4	J/mol	Constant
H_{RB}	−6.36 x 10^4	J/mol	Constant
E_A	3.64 x 10^4	J/mol	Constant
E_B	3.46 x 10^4	J/mol	Constant
C_p	3.2 x 10^3	J/kg/K	Constant
R	8.314	J/mol/K	Constant
ρ	1180.0	kg/m^3	Constant
	Initial design		
C_{Ai}	3118	mol/m^3	Input variable
C_{Bi}	342	mol/m^3	Input variable
T_i	300	K	Input variable
Q	1.71 x 10^6	J/min	Input variable
V	0.0391	m^3	Input variable
F	0.0781	m^3/min	Input variable
	Robust design		
C_{Ai}	3119.8	mol/m^3	Input variable
C_{Bi}	342.24	mol/m^3	Input variable
T_i	309.5	K	Input variable
Q	5.0 x 10^6	J/min	Input variable
V	0.05	m^3	Input variable
F	0.043	m^3/min	Input variable

discrepancy between our results and the previously published results is small (less than 0.2%) and likely due to differences in implementation of the solver for the system of equations.

Monte Carlo simulations were run using 10^6 samples to estimate the true standard deviation of the response of the CSTR due to the six noise factors. Then, six different methods were used to estimate the standard deviation of the response: (1) the quadrature technique using 25 samples; (2) HSS using 25 samples; (3) LHS using 25 samples; (4) QFM which required 33 samples; (5) HSS using 250 samples and (6) LHS using 250 samples.

Table 2 presents the results. The error of the quadrature technique as applied to the CSTR was about 5% for the initial design and improved substantially when the

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Table 2. Comparing the accuracy of sampling methods as applied to the continuous-stirred tank reactor

Sampling method	# of samples	$\mu(R_B)$	$\sigma(R_B)$	Error in estimate of σ (%)
		Initial design		
Monte Carlo	10^6	60.434	40.320	–
Quadrature	25	60.208	38.149	−5.4
HSS	25	57.988	39.315	−2.5
LHS	25	61.616	42.991	6.6
QFM	33	58.366	33.227	−17.6
Cubature	57	60.114	38.76	−3.9
HSS	250	59.903	40.217	0.3
LHS	250	59.770	39.791	−1.3
		Robust design		
Monte Carlo	10^6	50.894	15.242	–
Quadrature	25	50.735	15.169	−0.5
HSS	25	51.142	11.702	−23.3
LHS	25	49.676	16.993	11.5
QFM	33	34.915	9.725	−36
Cubature	57	50.621	15.453	1.4
HSS	250	50.985	15.532	1.9
LHS	250	50.438	15.702	3.0

design was made more robust. Given that there were nine randomly varying inputs, Theorem 2 suggested that the mean error would be about −0.5% and the standard deviation of error would be about 0.5 to 1%. These results are consistent with Theorem 2 at the robust set point, but the response to noise was unexpectedly challenging for the initial set point. HSS with 25 samples outperformed quadrature at the initial design, but then performed very poorly at the robust design. Cubature had slightly lower error than quadrature at the initial design, but quadrature performed much better than cubature at the robust design set point and also required about half as many function evaluations.

9.2. Case 2: LifeSat satellite

The engineering system in this case is a LifeSat satellite which was used to demonstrate the benefits of the Taguchi method (Mistree *et al.* 1993). The objective is to select a few key initial conditions at the start of a satellite de-orbit maneuver in order to have the satellite land near a specified target while minimizing the maximum acceleration and dynamic pressure during the de-orbit trajectory. The satellite itself is modeled as a point mass subject to gravitational, drag, and lift forces. The de-orbit sequence is as follows. First, the satellite is subjected to a

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Table 3. Parameters and their values in the LifeSat case study

Parameter	Value	Units	Description
h_s	8.563	Km	Constant
ρ_0	1.2	kg/m^3	Constant
g	9.81	m/s^2	Constant
R_0	6370	km	Constant
	Initial design		
Parameter	Mean	Standard Deviation	Distribution
Initial position: x	–1360.4 km	5000 m	Normal
Initial position: y	–4548.8 km	5000 m	Normal
Initial position: z	4427.5 km	5000 m	Normal
Vehicle mass	1560.4 kg	1.667%	Uniform
Atm. density	1.2 kg/m^3	10%	Normal
Drag coefficient	0.668	1.667%	Normal
Initial speed: V_x	–1559.1 m/s	0.667%	Normal
Initial speed: V_y	–5213.2 m/s	0.667%	Normal
Initial speed: V_z	–7168.8 m/s	0.667%	Normal
	Robust design		
Initial longitude	106.65^o	0.01^o	Normal
Initial latitude	43.783^o	0.1^o	Normal
Initial altitude	12,1920 m	250m	Normal
Vehicle mass	1460.0 kg	1.667%	Uniform
Atm. density	1.2 kg/m^3	10%	Normal
Drag coefficient	0.668	1.667%	Normal
Initial velocity	9846.5 m/s	0.667%	Normal
Initial flight path angle	–5.98^o	0.1^o	Normal
Initial azimuth	180^o	0.1^o	Normal

prescribed thrust to set it on a de-orbit path. The initial state of the satellite after this thrust is described by a three-dimensional position and a velocity vector. Next, the satellite proceeds through a freefall stage whereby it experiences the effects of gravity drag and lift forces until it contacts the earth's surface. The states of importance in the calculation of this trajectory are the landing position and a measure representative of the maximum force that the satellite experiences during free fall. The system is governed by three equations.

$$\boldsymbol{F}_{tot} = -m\left(\mu/R^2\right)\boldsymbol{e}_R + \frac{1}{2}\rho v_r^2 A_{ref} c_d \boldsymbol{e}_d, \tag{28}$$

$$\rho \approx \rho_0 \cdot \exp\left[-(h-h_o)/h_s\right], \tag{29}$$

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$$\mu = gR_0^2. \tag{30}$$

Table 3 provides a listing of physical constants and nine dispersed vehicle and environmental parameters (Mistree *et al.* 1993). We considered two different designs both described in the published case – one was an initial design and the other was an optimized robust design with greatly reduced variance in the landing coordinate.

In order to validate the simulation code, a verification study was performed. Mistree *et al.* (1993) found the landing position of −106.65° longitude and 33.71° latitude. We obtained −106.65° longitude and 33.69° latitude.

Monte Carlo simulations were run using 10^4 samples to estimate the true standard deviation of both landing longitude and latitude due to the nine noise factors. Then, six different methods were used to estimate the standard deviation of the response: (1) quadrature (Eqs. (4)–(6)) using $4n + 1$ or 37 samples; (2) HSS using 37 samples; (3) LHS using 37 samples; (4) QFM which required 33 samples; (5) HSS using 370 samples; and (6) LHS using 370 samples.

Tables 4 and 5 present the results. The error of the quadrature technique as applied to the LifeSat satellite was less than 2% for the initial design and robust design. Given that there were nine randomly varying inputs, Theorem 2 suggested that the mean error would be about −0.5% and the standard deviation of error would be about 0.5% to 1%. These results are generally consistent with Theorem 2 at both the robust set point and the initial set point. Quadrature outperformed

Table 4. Comparing the accuracy of sampling methods as applied to the LifeSat satellite (longitude)

Sampling method	# of samples	μ	σ	Error in estimate of σ
		Initial design		
Monte Carlo	10^4	−106.65	0.056	–
Quadrature	37	−106.65	0.056	0%
HSS	37	−106.65	0.0545	−2.7%
LHS	37	−106.65	0.0591	5.5%
QFM	33	−106.65	0.0536	−4.3%
HSS	370	−106.65	0.0556	−0.7%
LHS	370	−106.65	0.0563	0.5%
		Robust design		
Monte Carlo	10^4	−106.65	0.0077	–
Quadrature	37	−106.65	0.0078	1.3%
HSS	37	−106.65	0.0071	−7.8%
LHS	37	−106.65	0.0073	5.2%
QFM	33	−106.65	0.0053	−31.2%
HSS	370	−106.65	0.0077	0%
LHS	370	−106.65	0.0076	−1.3%

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Table 5. Comparing the accuracy of sampling methods as applied to the LifeSat satellite (latitude)

Sampling method	# of samples	μ	σ	Error in estimate of σ (%)
		Initial design		
Monte Carlo	10^4	33.5895	0.8260	–
Quadrature	37	33.5840	0.8122	–1.7
HSS	37	33.5231	0.8231	–0.4
LHS	37	33.5856	0.7088	–14.2
QFM	33	33.5815	0.5190	–37.2
Cubature	111	33.6101	0.6651	–19.5
HSS	370	33.5753	0.8262	0.02
LHS	370	33.5749	0.8719	5.6
		Robust design		
Monte Carlo	10^4	33.6992	0.2007	–
Quadrature	37	33.6979	0.2018	–0.5
HSS	37	33.7288	0.1698	–15.4
LHS	37	33.6936	0.2297	14.4
QFM	33	33.6978	0.1854	7.6
Cubature	111	33.6982	0.2225	9.8
HSS	370	33.7015	0.1893	–5.7
LHS	370	33.6979	0.1960	–2.3

HSS, LHS, and QFM with similar samples at both the initial design and the robust design. Cubature required three times as many function evaluations and yet performed less well than quadrature.

9.3. Case #3: I Beam

The engineering system in this case is an I beam which was used to demonstrate the advantages of dimension reduction integration in uncertainty analysis (Huang & Du 2005). The parameters in the model are depicted graphically in Figure 6.

The system is governed by the following three equations

$$Y = g(X) = \sigma_{\max} - S, \tag{31}$$

$$\sigma_{\max} = \frac{Pa(L-a)d}{2L \cdot I}, \tag{32}$$

$$I = \frac{b_f d^3 - (b_f - t_w)(d - 2t_f)^3}{12}, \tag{33}$$

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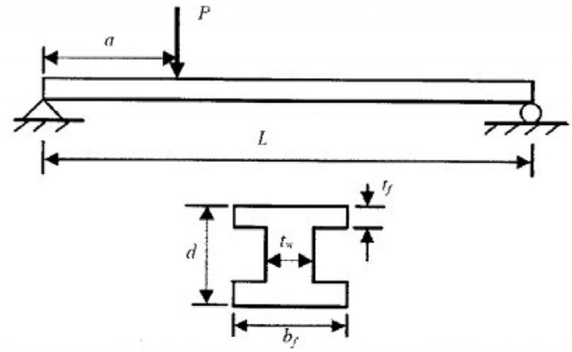

Figure 6. Parameters of an I-beam (adapted from Huang & Du (2005)).

Table 6. Parameters and their values in the I beam case study

Parameter	Mean	Standard Deviation
	Initial design	
P	6070	200
L	120	6
a	72	6
S	170,000	4760
D	2.3	1/24
b_f	2.3	1/24
t_w	0.16	1/48
t_f	0.16	1/48
	Robust design	
P	10,125	200
L	240	6
a	109	6
S	85,000	4760
D	4.6	1/24
b_f	4.6	1/24
t_w	0.32	1/48
t_f	0.52	1/48

Table 6 provides a listing of eight random variables which are taken directly from the published case study (Huang & Du 2005). We considered two different designs – one was an initial design from the published case and the other was an optimized robust design proposed here with greatly reduced variance in the output performance.

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To check that the model was correctly implemented, the results at both points were reproduced by Monte Carlo simulations with 10^6 trials each. Huang & Du (2005) found the first and second estimated moments about zero using 10^6 samples. The previously published value of the transmitted variance was 3.2137×10^8. We computed the transmitted variance of 3.2048×10^8. The discrepancy between our results and the previously published results is small (less than 0.3%).

Monte Carlo simulations were run using 10^6 samples to estimate the true standard deviation of the output performance due to the eight noise factors. Then, six different methods were used to estimate the standard deviation of the response: (1) quadrature (Eqs. (3) and (4)) using $4n + 1$ or 33 samples; (2) HSS using 33 samples; (3) LHS using 33 samples; (4) QFM which required 33 samples; (5) HSS using 330 samples and 6) LHS using 330 samples.

Table 7 presents the results of the case study. The accuracy of the quadrature technique as applied to the I-beam was excellent and generally as expected according to Theorem 2. The error was less than 1% and improved slightly as the design was made more robust. This level of accuracy was superior to any method using a comparable number of samples. However, if HSS was afforded 10 times the number of samples as quadrature, it could also provide excellent accuracy. Cubature required more than twice the function evaluations and

Table 7. Comparing the accuracy of sampling methods as applied to the I beam

Sampling method	# of samples	μ	σ	Error in estimate of σ (%)
		Initial design		
Monte Carlo	10^6	−19,825	17,902	–
Quadrature	33	−19,805	17,722	−1.0
HSS	33	−17,698	16,407	−8.4
LHS	33	−20,540	16,195	−9.5
QFM	33	−19,850	16,831	6.0
Cubature	73	−19,819	17,915	−0.1
HSS	330	−19,271	17,601	−1.7
LHS	330	−19,943	17,097	−4.5
		Robust design		
Monte Carlo	10^6	−19,818	5535.7	–
Quadrature	33	−19,825	5537.4	0.01
HSS	33	−18,969	4948.1	−10.6
LHS	33	−19,793	6003.3	8.5
QFM	33	−19,824	5470	−1.2
Cubature	73	−19,825	5541	0.1
HSS	330	−19,623	5418.2	−2.1
LHS	330	−19,829	5770.6	4.3

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performed better at the initial set point but worse than quadrature at the robust set point.

9.4. Case #4: 10-bar truss

The engineering system in this case is a linear-elastic 10-bar truss structure which was used to demonstrate the accuracy and efficiency of the univariate approximation method in higher-order reliability analysis (Rahman & Wei 2006). Two concentrated forces are applied at nodes 2 and 3 of the structure as indicated in Figure 7. The maximum displacement occurs at node 3 which is taken as the performance function of interest. Although the components of the truss behave linearly with applied load, the displacements of the structure are large enough to bring about significantly nonlinear behavior of the structure.

Table 8 provides a listing of physical constants and 10 random variables which are taken from the published case (Rahman & Wei 2006). We considered two different "designs" – one was an initial design given in the published case and the other was an optimized robust design proposed here with greatly reduced variance in the output performance.

To check that the model was correctly implemented, the failure probability of the 10-bar truss structure was reproduced by Monte Carlo simulations with 10^6 trials. Rahman found a failure probability of 0.1394 using 10^6 samples (Rahman & Wei 2006) and we computed 0.1392 using 10^6 samples. The discrepancy between our results and the previously published results are small (less than 0.2%).

Monte Carlo simulations were run using 10^6 samples to estimate the true standard deviation of the output performance due to the 10 noise factors. Then, six different methods were used to estimate the standard deviation of the response: (1) quadrature (Eqs. (4)–(6)) using $4n + 1$ or 41 samples; (2) HSS using 41 samples; (3) LHS using 41 samples; (4) QFM which required 33 samples; (5) HSS using 410 samples; and (6) LHS using 410 samples.

Table 9 presents the results. The error of the quadrature technique as applied to the 10-bar truss was around 3% for both the initial design and the robust design. Given that there were eight randomly varying inputs, Theorem 2 suggested that the mean error would be about -0.5% and the standard deviation of error would be about 0.5 to 1%. These results suggest that the 10-bar truss was somewhat

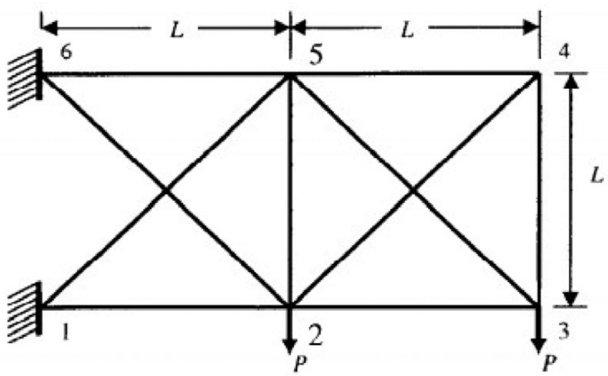

Figure 7. Parameters of a 10-bar truss (from Rahman & Wei (2006)).

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Table 8. Parameters and their values in the 10-bar truss case study

Parameter	Value	Units	Description
Young's modulus E	10^7	psi	Constant
Load P	10^5	lb	Constant
Length L	360	in	Constant
Initial design			
Parameter	Mean	Standard Deviation	
X_i, $i = 1, \ldots, 10$	2.5 in	0.5 in	
Robust design			
X_1	2.7272	0.5 in	
X_2	2.2727	0.5 in	
X_3	2.2727	0.5 in	
X_4	2.2727	0.5 in	
X_5	2.7156	0.5 in	
X_6	2.2727	0.5 in	
X_7	2.2727	0.5 in	
X_8	2.7500	0.5 in	
X_9	2.2727	0.5 in	
X_{10}	2.2727	0.5 in	

challenging case for quadrature. LHS and HSS outperform quadrature if they are afforded 10 times number of samples but are substantially less reliable if they have to use the same number of samples as quadrature. Note that in this case study, the standard deviation of noise factor is 20% of the mean whereas in the model-based evaluation of Section 4, the standard deviation of noise factor is 10% of the mean. Cubature required more than three times as many function evaluations and had similar performance as quadrature.

9.5. Case 5: operational amplifier

The engineering system in this case is an operational amplifier (op amp) which was used by to demonstrate the use of orthogonal arrays for robust design with computer simulations (Phadke 1989). The circuit is presented in Figure 7. The op amp is to be manufactured on a single board using 15 circuit elements whose parameters are to be chosen so that the offset voltage of the circuit is consistent despite manufacturing variations. There are 21 noise factors which affect the offset voltage (20 characterizing the circuit elements and one for the operating temperature) as shown in Table 10. Following the example of Phadke, we modeled some of the noise factors as correlated and some as independent. Phadke defined sliding levels to use in an L36 orthogonal outer array. We calculated the covariance matrix for the noise exhibited in the L36 array, and then ran various sampling schemes

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Table 9. Comparing the accuracy of sampling methods as applied to the 10-bar truss

Sampling method	# of samples	μ	σ	*Error in estimate of σ* (%)
		Initial design		
Monte Carlo	10^6	16.3225	1.6334	–
Quadrature	41	16.3145	1.5913	–2.6
HSS	41	16.5797	1.7042	4.3
LHS	41	16.3307	1.5419	–5.6
QFM	33	16.3329	1.7685	8.3
Cubature	133	16.3138	1.5662	–4.1
HSS	410	16.3947	1.6570	1.4
LHS	410	16.3199	1.6824	3.0
		Robust design		
Monte Carlo	10^6	16.333	1.5102	–
Quadrature	41	16.3225	1.4670	–2.9
HSS	41	16.6898	1.5784	4.5
LHS	41	16.3848	1.9018	25.9
QFM	33	16.3468	1.6697	10.6
Cubature	133	16.3256	1.4784	–2.1
HSS	410	16.4137	1.5281	1.2
LHS	410	16.3343	1.5529	2.8

assuming the same covariance. Phadke also defined some noise factors as lognormally distributed. We adapted different sampling methods by transforming those input variables and then treating the transformed inputs as normally distributed variates. We considered two different designs, an initial design and a robust design as described in Table 10 (Phadke 1989).

We developed a simulation of the op amp circuit based on an Ebers-Moll model of the transistors. To check that the model was correctly implemented, the results were checked against Phadke's published figures for the L36 outer array. Once the simulation was verified, we tested sampling techniques on it.

Monte Carlo simulations were run using 3×10^4 samples to estimate the true standard deviation of the response of the op amp due to the 21 noise factors. Then, four different methods were used to estimate the standard deviation of the offset voltage: (1) the quadrature technique (Eqs. (3)–(5)) using $2m + 1$ or 43 samples; (2) HSS using 43 samples; (3) LHS using 43 samples; (4) HSS using 430 samples; and (5) LHS using 430 samples.

Table 11 presents the results of the case study. The accuracy of the quadrature technique as applied to the op amp was excellent beginning at less than 1% error and improving slightly as the design was made more robust. Given that there were 19 randomly varying inputs, Theorem 2 suggested that the accuracy would be

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Table 10. Noise factors in the op amp case study, means and standard deviations

Parameter	Mean	Tolerance (%)	Units
RFM	71	1	kΩ
RPEM	15	21	kΩ
RNEM	2.5	21	kΩ
CPCS	20	6	μA
OCS	20	6	μA
RFP	RFM	2	Ω
RIM	RFM/3.55	2	Ω
RIP	RFM/3.55	2	Ω
RPEP	RPEM	2	Ω
RNEP	RNEM	2	Ω
AFPM	0.9817	2.5	–
AFPP	AFPM	0.5	–
AFNM	0.971	2.5	–
AFNP	AFNM	0.5	–
AFNO	0.975	1	–
SIEPM	3.0E-13	Factor of 7	A
SIEPP	SIEPM	Factor of 1.214	A
SIENM	6.0E-13	Factor of 7	A
SIENP	SIENM	Factor of 1.214	A
SIENO	6.0E-13	Factor of 2.64	A
TKLEV	298	15	°K

improved compared to the other cases which is what we observed. The level of accuracy attained by quadrature was superior to any method using a comparable number of samples. However, if HSS was afforded 10 times the number of samples as quadrature, it could also provide excellent accuracy. Unlike the other four systems simulated, QFM was not run on the op amp. The method could not be scaled to accommodate the large number of noise factors. Instead an L36 orthogonal array is presented as a basis of comparison. The L36 provided good results for this system, but not as good as the quadrature technique. The cubature method required more than 10 times the function evaluations and performed less well than quadrature.

9.6. All the case studies as a set

The set of case studies presented here can be studied as a set. There were five engineering systems and six different responses. For each response, there were an initial and a robust design making 12 case studies in total. Given the accuracy of each method applied across all the cases, it is possible to construct an empirical cdf

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Table 11. Comparing the accuracy of sampling methods as applied to the operational amplifier

Sampling method	# of samples	μ	σ	Error in estimate of σ (%)
Initial design				
Monte Carlo	3×10^4	−2.994	32.674	–
Quadrature	43	−2.7899	32.738	0.2
HSS	43	−16.041	22.265	−31.6
LHS	43	−3.796	28.263	−13.5
HSS	430	−4.433	33.187	1.6
LHS	430	−2.758	33.008	1.0
Cubature	507	−2.763	30.048	−8.0
L36	36	−2.862	33.282	1.9
Robust design				
Monte Carlo	3×10^4	1.727	19.988	–
Quadrature	43	−1.611	20.014	0.1
HSS	43	−8.378	12.963	−35.1
LHS	43	−2.266	17.606	−11.9
HSS	430	−2.396	20.14	0.8
LHS	430	−1.607	20.414	2.1
Cubature	507	−1.610	18.672	−6.6
L36	36	−1.653	20.259	1.4

of its accuracy. These are presented in Figure 8 with the model-based cdf for the $4m + 1$ quadrature technique as previously presented in Figure 5.

A principal observation is that, for the $4m + 1$ quadrature technique, the empirical cdf largely matches the model-based cdf. In the range of 3%–5% accuracy, the empirical cdf indicated a somewhat lower probability than the model-based cdf, but this deviation is within the 95% confidence range predicted by the model when only 12 samples are used to construct a cdf (the 95% range is not depicted since Figure 6 is already very dense). Note that the case studies make no assumption of polynomial response behavior. Therefore we submit that the model-based approach to evaluating the accuracy of the sampling methods has passed a stringent test.

Another important set of conclusions arise from comparing the empirical cdfs for the different methods. As in the model-based evaluation, quadrature substantially outperforms the previously available methods when they employ a comparable number of simulations. For the case studies, it appears that if 10 times the number of simulations can be run, then quadrature provides slightly better results.

Also, note that in four out of five case studies, the accuracy of quadrature is better for the robust design than for the initial design. It is not yet clear that this phenomenon is reliable, but it would be useful if it were. As the outer optimization

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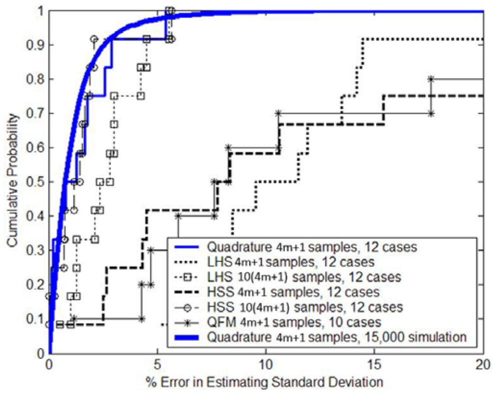

Figure 8. Empirical cumulative density functions based on the set of case studies. The model-based cumulative density functions of the $4m + 1$ quadrature technique is provided for comparison.

loop begins to hone in on promising design candidates, the ability to make finer distinctions becomes more valuable.

Overall, the case studies as a set are consistent with the principal claims from the model-based evaluation. The quadrature technique enables a 10-fold reduction in the number of computational simulations needed for robust design while providing reasonable accuracy. In addition, the accuracy of the method usually improves as the design is made more robust which should be advantageous when the method is used as an inner loop of a robustness optimization procedure.

10. Conclusions

This paper provides an alternative tool for practitioners to efficiently estimate transmitted variance as part of Robust Parameter Design. This tool is based on Hermite–Gaussian quadrature which, by exploiting the property of hierarchy and compromising slightly on accuracy and bias, greatly reduces the number of samples needed and scales linearly with the number of variables. This paper provides an analysis of the accuracy of the estimated transmitted variance using the quadrature-based method for separable polynomial response systems. It is verified that the method gives exact transmitted variance if the response is up to a fourth-order separable polynomial response. Closed form expressions were derived for the error as well as for the statistical properties of the error (i.e., the mean and variance of error).

The advantages of the quadrature-based method were demonstrated by means of hierarchical probability models and a set of case studies. For typical populations of problems, it is shown that the method has good accuracy, providing less than 5% error in 90% of the applications. The proposed method provides much better accuracy than LHS or HSS, assuming these techniques are also restricted to using $4m + 1$ samples. Only if Hammersley Sequence Sampling is afforded at least 10 times the number of samples, can it provide approximately the same degree of accuracy as the quadrature technique.

The limitations of the quadrature-based method should be emphasized. The theorems and model-based evaluations in this paper are predicated on the

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assumption that the noise factors are all normally distributed and probabilistically independent. To accommodate correlated noise factors, a linear transformation can be applied to the noise variables to create a set of uncorrelated noise factors before applying the equations in this paper. This approach was used in the op-amp case study and it was effective in that application. More generally, the Mahalanobis transformation will serve to create a set of independent random variables from a set of normally distributed, correlated random variables (Härdle & Simar 2007). However, it should be noted that the transformed, uncorrelated noise factors will not always be probabilistically independent except under particular assumptions, for example, when the noise factors are all normally distributed. We have not yet determined how well the proposed quadrature method will work on correlated variables that depart significantly from a normal distribution.

It's an interesting fact that the quadrature-based method had improved accuracy at the robust set point (as compared to the initial design) in most of the case studies. This potential regularity has yet to be verified and would require more case studies to develop confidence in its existence and reliability. However, it seems reasonable that as a system becomes more robust to a set of noise factors, its response to noise also becomes more nearly separable. For a set point to exhibit substantial robustness as compared to other set points, the response surface (to noise factors, not control factors) has to be relatively flat, relatively smooth, and nearly devoid of salient features. It stands to reason that response surfaces matching this description might also be separable in their response to noise. If so, this would be an auspicious development for the quadrature method. As the robust design process searches for robust set points, it also improves the degree to which the assumptions needed for quadrature are satisfied.

It is hoped that the advantages of the quadrature-based method will prove helpful for engineering designers facing the demands of real-world pressures such as time and resource limitations. The proposed quadrature-based method adds value to the practitioner's toolbox. When practical engineering problems have less separability and smaller numbers of input variables, a cubature method might be a reasonable choice. A cubature method such as proposed by Lu & Darmofal (2005) will afford advantages when there are practically significant noise by noise interactions. The meta-model based approach proposed by Tan & Wu (2012) may offer advantages when a Gaussian process model can closely fit the true underlying response of the engineering system. However, when practitioners face engineering problems with larger numbers of input variables, the quadrature-based method can estimate the transmitted variance efficiently and accurately as compared to other approaches. The developments in this paper also provide *a priori* error estimates that appear to be reliable, so the method can be applied with confidence.

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