A Quadrature-based Technique for Robust Design with Computer Simulations

by

Yiben Lin

M.S. in Department of Aeronautics and Astronautics,
Massachusetts Institute of Technology (2003)

Submitted to the Department of Aeronautics and Astronautics
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

at the

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

June 2007

Author ....
Department of Aeronautics and Astronautics
March 7, 2007

Certified by ....
Daniel D. Frey
Associate Professor of Mechanical Engineering and Engineering Systems
Thesis Supervisor

Certified by ....
David Darmofal
Associate Professor of Aeronautics and Astronautics
Committee Chair

Certified by ....
Christopher Magee
Professor of Mechanical Engineering and Engineering Systems
Committee Member

Accepted by ....
Jaime Peraire
Professor of Aeronautics and Astronautics
Chair, Committee on Graduate Students

A Quadrature-based Technique for Robust Design with Computer Simulations

by
Yiben Lin

Submitted to the Department of Aeronautics and Astronautics
In partial fulfillment of the requirements for the degree of
DOCTOR OF PHILOSOPHY

Abstract

This thesis presents a method for estimating transmitted variance to enable robust parameter design in computer simulations. This method is based on the Hermite-Gaussian quadrature for a single input. It is extended to multiple variables, in which case, for simulations with n randomly varying inputs, the method requires $4n+1$ samples.

For situations in which the polynomial response is separable, it is proven that 1) the method gives exact transmitted variance if the response is up to a fourth-order separable polynomial response and 2) the error of the transmitted variance estimated by the method is smaller than zero if the response is a fifth-order separable polynomial response.

For situations in which the polynomial response is not separable, two probability models based on the effect hierarchy principle are used to generate a large number of polynomial response functions. The proposed method and alternative methods are applied to these polynomial response functions to investigate accuracy. For typical populations of problems, it is shown that the method has good accuracy, providing less than 5% error in 90% of cases. The proposed method provides much better accuracy than Latin Hypercube Sampling or Hammersley Sequence Sampling assuming these techniques are also restricted to using $4n+1$ samples. Hammersley Sequence Sampling requires at least ten times the number of samples to provide approximately the same degree of accuracy as the quadrature technique. A cubature method provides slightly better accuracy than the proposed method, though it requires n^2+3n+3 samples.

As an independent check on these results, simulations of five engineering systems are developed and 12 case studies are conducted. Although the predicted accuracy in case-based evaluations is somewhat lower, the data from the case-based evaluations are consistent with the results from the model-based evaluation.

Thesis Supervisor: Dr. Daniel D. Frey

Title: Associate Professor of Mechanical Engineering and Engineering Systems

Acknowledgements

I would like to thank my advisor, Prof. Daniel D. Frey for his encouragement and guidance, without his help and advise this thesis would not exist.

I also thank the other members of my thesis committee. Prof. David Darmofal was always quick to grasp what I had done and point out important things on which I should focus. Prof. Christopher Magee offered helpful assistance throughout. I also would like to thank Prof. Richard Larson and Dr. Sudijanto for taking time out from their busy schedules to serve as external thesis readers.

I would like to thank my office mates for their friendship, encouragement, and assistance through the pass four years, Hongren Wang, Xiang Li, Jagmeet Singh, Rajesh Jugulum, Troy Savoie, Chad Foster, Nandan Sudarsanam, Benjamin Powers.

Finally and most of all, I wish to thank my wife Tao, my parents Moudao and Aiying, My three sisters Qiong, Zhang and Fang, and my brother Jijun for their constant support.

Contents

1 Introduction

1.1 Background. 13

1.2 Robust Design. 15

1.3 Robust Design with Computer Experiments. 17

1.4 Computational Burden of Robust Design. 19

1.5 Sampling Methods. 21

1.5.1 Latin Hypercube Sampling. 21

1.5.2 Hammersley Sequence Sampling. 21

1.5.3 Quadrature and Cubature Sampling. .22

1.6 Motivation and Scope of Thesis. 22

2 Quadrature Formula for Multi-variable Polynomial Systems

2.1 Single Variable Hermite-Gaussian Formula. 25

2.2 Quadrature Formular for Multiple Variables. 27

3 The Comparison between the Quadrature-based Method and Sensitivity-based Method. 35

4 Model-based Evaluation for Un-Separable Polynomial Systems

4.1 The Third-Order Un-Separable Polynomial Model-based Evaluation. 39

4.2 Higher-Order Un-Separable Polynomial Model-based Evaluation. 44

5 Case Studies

5.1 Continuous-Stirred Tank Reactor. 51

5.2 Ten Bar Truss. 55

5.3 I-Beam. 59

5.4 LifeSate Satellite. 62

5.5 Op-Amp. 64

5.6 All the Cases as a Set. 67

6 Conclusions. 71

7 Reference. 73

List of Figures

Figure 1-1: Deterministic Analysis. 14

Figure 1-2: Probabilistic Analysis. 14

Figure 1-3: Nonlinearity of output response to inputs. 16

Figure 1-4: An I Beam. 17

Figure 1-5: Schematic description of robust design including a sampling loop embedded within an optimization loop. 18

Figure 2-1: Five point Hermite-Gauss Quadrature applied to an arbitrary function. . . 25

Figure 2-2: Sampling scheme for a system with three noise factors (n=3) and using the $4n$+1 rule. 27

Figure 4-1: Cumulative probability versus error in estimating transmitted variance for six different sampling procedures. 43

Figure 4-2: Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to populations of 5th order polynomials of four to eight variables (d=4~8) whose polynomial coefficients decrease geometrically with order at rate $\sqrt{r}$ =0.2 for single factor effects and at a faster rate (r_{INT}/r=0.2) for interaction effects. 48

Figure 5-1: Continuous-Stirred Tank Reactor. 52

Figure 5-2: LifeSat Satellite. 57

Figure 5-3: An Ten-Bar truss structure. 62

Figure 5-4: Differential Op Amp Circuit Diagram. 66

Figure 5-5: Empirical cumulative density functions based on the set of case studies. The model-based cumulative density functions of the $4n$+1 quadrature technique is provided for comparison. 68

Figure 5-6: Empirical cumulative density functions based on the set of case

studies. The model-based cumulative density functions
is provided for comparison. 69

Figure 6-1: The comparison of the quadrature-based method, cubature,
and SOSM. 72

List of Tables

Table 5-1: Parameters and their values in the CSTR case study. 53
Table 5-2: Comparing the accuracy of sampling methods as applied to the continuous-stirred tank reactor. 54
Table 5-3: Parameters and their values in the LifeSat case study. 57
Table 5-4: Comparing the accuracy of sampling methods as applied to the LifeSat Satellite (Longitude). 58
Table 5-5: Comparing the accuracy of sampling methods as applied to the LifeSat Satellite (Latitude). 59
Table 5-6: Parameters and their values in the I beam case study. 61
Table 5-7: Comparing the accuracy of sampling methods as applied to the I beam. 61
Table 5-8: Parameters and their values in the Ten-Bar Truss case study. 63
Table 5-9: Comparing the accuracy of sampling methods as applied to the ten-bar truss. 64
Table 5-10: Noise factors in the op-amp case study, means and standard deviations. .66
Table 5-11: Comparing the accuracy of sampling methods as applied to the operational amplifier. 67

Chapter 1

Introduction

1.1 Background

Many design and verification decisions demand the use of physics-based mathematical models. For example, these mathematical models could be a representation of a structural problem, a fluid flow problem, or an electrical circuit problem. Most often, these models are very complex because they often involve a system of partial differential equations and multiple parameters. Hence, we have to resort to computer codes to provide approximate solutions instead of analytical solutions to the system of partial differential equations. Currently computer modeling applied in a deterministic fashion is being employed in product development.

The inputs of a deterministic model are typically nominal or worst-case values. Examples of inputs are nominal values of dimensions, loads and materials. The outputs are point estimates of performance functions such as deflection, life, and voltage. A safety margin can be derived from the point estimate of the outputs. A designer with a deterministic model should choose a larger safety margin design for better reliability. As shown in Figure 1.1, Design B, which has a larger safety margin than Design A, should be chosen.

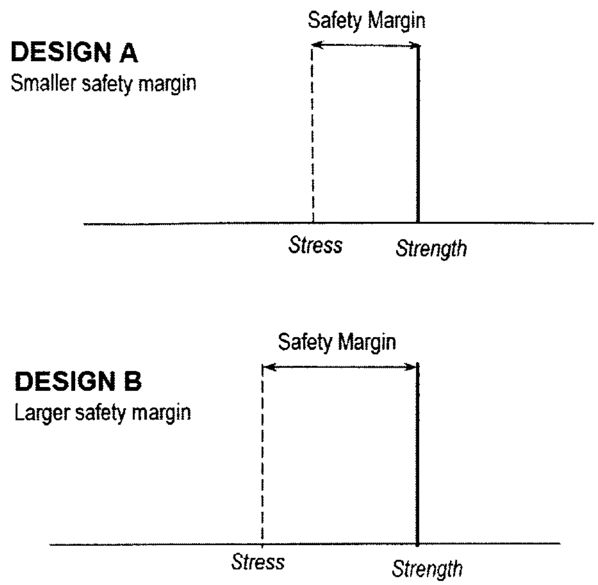


Figure 1.1 Deterministic Analysis.

However, this might be a wrong choice if the output variation is considered. As shown in Figure 1.2, an output such as stress has a distribution due to variations of inputs. Product failure occurs when the output stress is greater than the strength. It is obvious that Design A is less likely to fail than Design B. In other words, Design A has a higher reliability than design B, even though Design A has a smaller safety margin. Therefore, ignoring variations of inputs during the design process can sometime leads to a design with lower reliability.

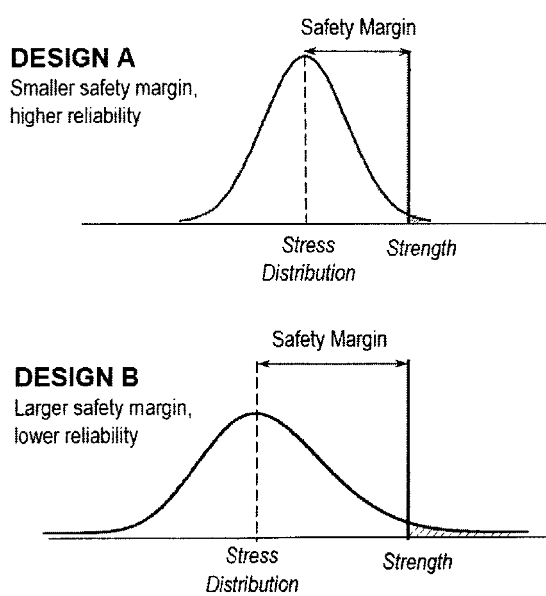


Figure 1.2 Probabilistic Analysis.

In probabilistic methods, output mean and variance can be obtained by either a sensitivity-based method or a sampling method. The sensitivity-based method approximates the input-output relation $y(z)$ by a low-order Taylor series and computes the approximate mean and variance from the approximated function.

$$y(z) \approx y(\bar{z}) + \sum_{i=1}^{n} \frac{\partial y_i}{\partial z_i} \Delta z_i \tag{1.1}$$

$$\mu_y = y(\bar{z}_1, \bar{z}_2, \ldots, \bar{z}_n) \tag{1.2}$$

$$\sigma_y^2 = \sum_{i=1}^{n} \left(\frac{\partial y_i}{\partial z_i} \right)^2 \sigma_{z_i}^2 \tag{1.3}$$

where

$$\frac{\partial y}{\partial z_i} \approx \frac{y(\bar{z}_1, \bar{z}_2, \ldots, \bar{z}_i + \alpha\bar{z}_i, \ldots, \bar{z}_n) - y(\bar{z}_1, \bar{z}_2, \ldots, \bar{z}_n)}{\alpha\bar{z}_i} \text{ and } \alpha = 0.01\text{~}0.05 \tag{1.4}$$

Equation 1.1 shows a first-order Taylor approximation of a separable function $y(z)$. The mean and variance of $y(z)$ can be obtained from Equations 1.2 and 1.3. Here, only the diagonal elements of the Jacobian matrix $\frac{\partial y_j}{\partial z_i}$ are non-zero. This method requires the calculation or approximation of the derivatives of $y(z)$ as shown in Equations 1.4, which can involve significant computational effort and numerical error (e.g., James and Oldenburg 1997, Malkawi, Hassan, and Abdulla 2000). When $y(z)$ is highly nonlinear, the error in estimating the output mean and variance might not be negligible. It may then be necessary to switch to a sampling method to obtain the output distribution by repeatedly running the deterministic model, given different input values from input distributions. In order to successfully apply a sampling method, the distributions of input variables must be specified. This can be done using expert knowledge of the product or past experience. Next, a sampling method, for example, Monte Carlo sampling, can be used to pick up input values from their distributions. The deterministic model is used to obtain the corresponding output values which form the distribution of outputs for assessing the level of reliability of the product. Although probabilistic methods can provide the output distribution for accessing the reliability, it cannot give design direction to the designer. More direct design input can be obtained through use of robust parameter design methodology.

1.2 Robust 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; Wu and Hamada 2001). The variables that affect a product's response are classified into *control* factors whose nominal settings can be specified by the designer and *noise* factors that cause unwanted variations in the system response. In order to achieve a robust design, the designer needs to identify settings of control factors to minimize the output's deviation from the target value. This can be achieved by exploiting nonlinearity of the product's input-output relation. Usually the input-output relation of a typical engineering system is a nonlinear function. Hence, it is possible to find many combinations of settings of control factors that can give the desired target value with different variations. In robust design, significant reduction of the output variation can be achieved by simply changing the settings of control factors from design point A to design point B, as illustrated in Figure 1.3. This change has the advantage that it does not require the elimination of the source of variation. It also makes it possible to achieve robust products without adding manufacturing costs.

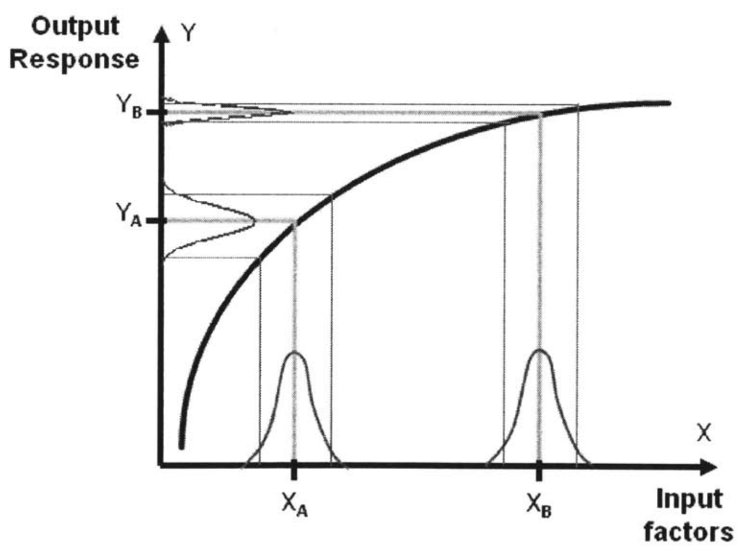


Figure 1.3 Nonlinearity of output response to inputs.

Consider a simple engineering system, the "I beam." This is a common example used in the uncertainty analysis literature (Huang 2005, Wang 2004) and is used here to illustrate robust design. The output is the safety range, which is the difference between the maximum stress on the beam and the strength of the beam. The inputs that affect the safety range are the load P, the beam strength S, and the geometric parameters of the beam, as shown in Figure 1.4. All inputs are random variables with normal distributions. Hence, for robust design, the control factors are the eight nominal values of the inputs. These nominal values can be specified by designers. The noise variables are the corresponding variations around the nominal values. These variations cause unwanted variation of the safety range of the I beam. The objective of robust design of the I beam is to choose the settings of the load P, the beam strength S, and the geometric parameters of the I beam such that the variation of the safety range around the set point is kept to a minimum. This objective can be achieved by exploring the nonlinearity of the safety range and the inputs.

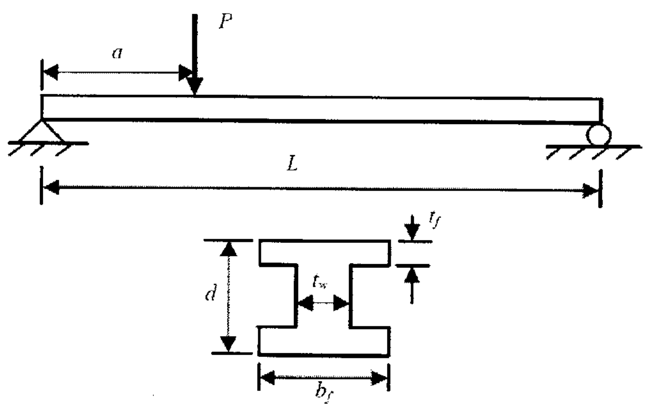


Figure 1.4 An I Beam (Adapted from Huang 2005).

1.3 Robust Design with Computer Experiments

In the past, robust design was typically done utilizing results from laboratory experiments. However, many products and processes are so complex that laboratory experiments with robust design are too time consuming or too expensive. As a result, robust design is increasingly performed using computer models of the product or process rather than laboratory experiments. With the steady and continuing growth in computer power and speed, computer models can provide significant advantages in the cost and speed of robust design.

Robust design with computer experiments is often accomplished using a strategy employing two nested loops as depicted in Figure 1.5: 1) an inner sampling loop, and 2) an outer optimization loop (Kalagnanam and Diwekar 1997; Du and Chen 2002; Li and Sudjanto 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 is the same as the probabilistic model, which can be used to estimate robustness, and the outer optimization loop serves to improve the design, often by decreasing the variance of model output.

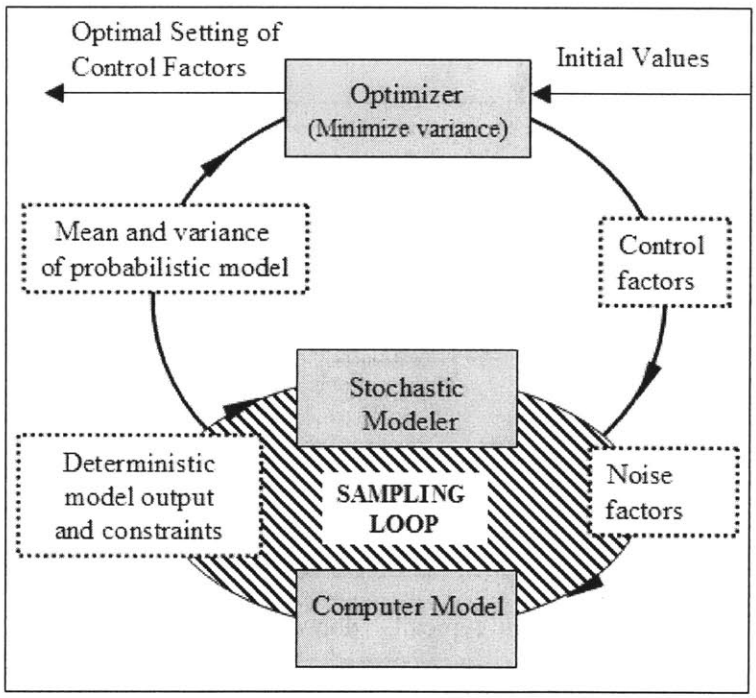


Figure 1.5 Schematic description of robust design including a sampling loop embedded within an optimization loop (Adapted from Kalagnanam and Diwekar 1997).

Again, take the I beam for an example. For each setting of control factors (each setting of nominal values of eight inputs), a sampling loop is needed to calculate the variation of the output (safety range) to assess the robustness. Then, the variation of the safety range is used as the input for the optimization loop to search for the optimum setting of control factors, which may lead to minimal variation of the safety range of the I beam.

Although random variations in noise factors can be simulated in a computer, the results of computer models generally lack pure experimental error as well as complex environment effects (which may also be missed experimentally). Therefore, it is generally acknowledged that the techniques for robust design via computer models ought to be different from 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. Background on this subject is provided from various perspectives by Santner et al., 2003, Giunta, et al., 2003, and Simpson et al. 2001.

1.4 Computational Burden of Robust Design

As mentioned before, robust design includes an inner sampling loop to estimate robustness and an outer optimization loop to improve robustness. Hence, a difficulty of robust design with computer simulation is that its resource demands typically scale as the *product* of the demands of the inner and outer loops. Assuming M minutes per run for the I beam simulation, a simulation of N samples would require M*N minutes to obtain the variation of the safety range to assess the robustness in the inner sampling loop. Further assuming K iterations are needed in the outer optimization loop to find the setting of control factors with minimal variation of the outputs, the expense of robust design would require M*N*K minutes.

The computational cost of some complex models of practical engineering systems is non-trivial for even a single run. For instance, aerodynamic or finite element analyses are often implemented in complex computer codes that require minutes to hours on the fastest computers.

Here are a few computational challenge examples from the literature:

Example 1: Piston Slap Noise

Li and Sudjianto (2005) describe a piston slap noise model for reducing the unwanted engine noise resulting from piston secondary motion. The output variable is the piston slap noise and the inputs are clearance between the piston and the cylinder liner, location of peak pressure, skirt length, skirt profile, skirt ovality, and pin offset. The piston system model includes a multi-body dynamics model, flexible body model, and rigid body model. The computational time for a single piston slap noise simulation could take 24 hours.

Example 2: Automotive Crash Simulation

Koch, Yang, and Gu (2004) describe an automotive crashworthiness model for vehicle structural design. The inputs are velocity of impact, mass of vehicle, angle of impact, and mass/stiffness of barrier, and many other uncertain parameters. The objective is to design the vehicle structure to absorb and manage the crash energy. Computer simulation involving finite element models is used for crash analysis. The finite element models can use upwards of 150,000 elements. It can often take 20, or even as much as 150 or more hours, for the crash simulation on a full passenger car.

Example 3: Assembly of the Dashboard Panel

It is reported that it takes Volvo 40 minutes to run one simulation for the sheet metal assembly of the dashboard panel (Dahlstrom 2005).

Therefore, in the context of complex models for practical engineering systems, it may be very difficult to collect a large sample to assess robustness in the inner sampling loop, let alone the probabilistic optimization to improve the robustness. For instance, at one hour per run, 1000 simulations in the inner sampling loop would require more than 41 days to assess the robustness. Assuming that, on average, 50 iterations are needed in the outer optimization loop to improve robustness, even with parallel processing, the expense of computer simulation prohibits probabilistic optimization.

Thus, the meta-model approach has been widely used in practice to overcome the computational complexity (e.g., Simpson et al. 2001; Booker et al. 1999; Hoffman, Sudjianto et al., 2003; Du et al. 2004). Meta-model, also called "model of model" or "surrogate model", denotes a user-defined cheap-to-compute function which is an approximation of 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 (e.g., Ye, Li, and Sudjianto 2000, Jin, Chen, and Simpson 2000).

As a complementary and possibly alternative approach, one may develop efficient sampling methods to reduce the computational cost of the inner sampling loop for practical and efficient robust design. This thesis is intended to help greatly reduce the resource demands of the inner sampling loop.

1.5 Sampling Methods

A lot of research has been done on how to assess robustness using sampling methods. Three of the most promising sampling methods that can be used to assess robustness in the inner loop are reviewed in the next three sections.

1.5.1 Latin Hypercube Sampling

Latin Hypercube Sampling (LHS) is a stratified sampling technique which can be viewed as an extension of Latin square sampling and a close relative of highly fractionalized factorial designs (McKay et al. 1979). In order to use LHS to select p samples from n input variables, the distribution of each input variable is subdivided into non overlapping intervals (p bins) of equal probability. Hence, the partitioning yields a total of p^n bins. LHS ensures that (1) each sample is randomly placed inside a bin, and (2) each input variable has all portions of its distributions uniformly represented by input values. The second property (often referred to as a "projective" property) is especially advantageous when only a few of the many inputs turn out to contribute significantly to the output variance. McKay et al. (1979) proved that for large samples, LHS provides smaller variance in the estimators than simple random sampling as long as the response function is monotonic in all the noise factors. However, there is also evidence that LHS often provides little practical advantage over simple random sampling if the response function is highly non-linear (Giunta *et* al. 2003). Two often-cited shortcomings associated with LHS are non-uniform properties on a k-dimensional unit hypercube (for k input variables) and probabilistic bounds due to more than one possible sampling meeting the LHS criteria.

1.5.2 Hammersley Sequence Sampling

An innovation called Hammersley Sequence Sampling (HSS) may provide significant advantages over LHS (Kalagnanam and 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. In an engineering application with six noise factors, HSS converged to 1% accuracy up to 40 times faster than LHS (Kalagnanam and Diwekar, 1997). However, for higher dimensions, the HSS points are not evenly dispersed. That means HSS's low discrepancy and good space-filling properties only exist for smaller-dimensional problems. The sample mean and sample variance obtained using HSS might have larger error for higher-dimensional problems.

1.5.3 Quadrature and Cubature

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 and Rabiniwitz (1993) and Cools (1999) for reviews. More recently, Lu and Darmofal (2005) developed a new cubature method for Gaussian weighted integration was developed that scales better than other, previously published cubature schemes. If the number of uncertain factors in the inner loop is n, then the method requires n^2+3n+3 samples. The new rule provides exact solutions for the mean for polynomials of fifth degree including the effects of all multi-factor 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 cuabature 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.

1.6 Motivation and Scope of Thesis

The motivation for this thesis is that available sampling schemes 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 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 and accuracy. All of these considerations suggest a need for techniques requiring a very small number of samples. This need motivated the new technique described in the next chapter.

This thesis extends previous research results on the quadrature–based sampling method in the Robust Design group at MIT (e.g., Reber 2004). Previously, Frey and Reber (Reber 2004) generalized the one dimensional quadrature rule to n-dimension case and derived a transmitted variance formula. The transmitted variance formula was applied to a few case studies to illustrate the accuracy and efficiency of the quadrature-based method. This quadrature–based sampling method is intended to evaluate multi-dimensional integration.

This thesis advances the quadratue-based method in the following area:

1) Correcting the transmitted variance formula for the quadrature-based method (Chapter 2),
2) Comparing the quadrature-based method with the sensitivity-based method for separable multi-variable polynomial systems and makes suggestions for the sensitivity-based method to improve its accuracy (Chapter 3),
3) Comparing the quadrature-based method to alternative methods based on two probability models of un-separable polynomial systems (Chapter 4), and
4) Illustrating the advantages of the quadrature-based method using five practical engineering systems. (Chapter5).

Chapter 2

Quadrature-Based method for Multi-variable Polynomial Systems

2.1 Single Variable Hermite-Gaussian 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 (HGQ). 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 2.1 describes the concept as applied to an arbitrary function $y(z)$.

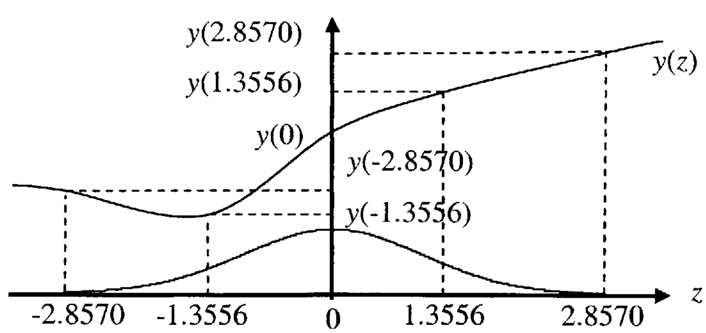


Figure 2.1 Five-point Hermite-Gauss Quadrature applied to an arbitrary function

The function is sampled at five points. One sample is at the mean of the variable z which is zero for a standard normal variate. The other four samples are distributed symmetrically about the origin at prescribed points. The values of the function $y(z)$ are 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 1966). The five-point Hermite-Gaussian quadrature formula for estimating the mean $E[y(z)]$ is

$$Q[y] = y(\bar{z}) + \sum_{j=1}^{4} \alpha^{(j)} \left[y\left(D^{(j)} + \bar{z}\right) - y(\bar{z}) \right] \tag{2.1}$$

where $\bar{z}$ is the mean of the variable z, $\boldsymbol{\alpha}_{4\times1} = (0.2221 \quad 0.0113 \quad 0.0113 \quad 0.2221)^T$, and $\mathbf{D}_{4\times1} = (-2.857 \quad -1.3556 \quad 1.3556 \quad 2.857)^T$.

Estimating variance also involves computing an expected value, namely $E\left[\left(y(z) - E[y(z)]\right)^2\right]$. By using Equation 2.1 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 because the function being integrated includes the square of $y(z)$.

Generally, a N-point Hermite-Gaussian quadrature formula with a set of $(\boldsymbol{\alpha}, \mathbf{D})$ can give the exact mean if $y(z)$ is a polynomial of degree $2N-1$ or less. When used recursively to compute the variance, the order of the polynomials integrated exactly drops by a factor of two if N is even and slightly more if N is odd, in which case it drops by a factor of $(2N-1)/(N-1)$.

2.2 The Quadrature-based Method for Multiple Variables

In the multi-dimensional case, estimation of integrals becomes more complex. A variety of cubature formulae for Gaussian weighted n dimensional integrals have been derived (Stroud 1971). These cubature techniques all scale poorly with the dimensionality of the integral despite recent improvements. To circumvent the problem of scaling in multidimensional integrals, it is proposed that a one-dimensional quadrature rule can be adapted to n-dimensional problems.

A graphical depiction of the design for three standard normal variables (n=3) and using $4n+1$ samples is presented in Figure 2.2. The sampling scheme is composed of one center point and 4 axial runs per variable. Thus the sampling pattern is similar to a star pattern in a central composite design.

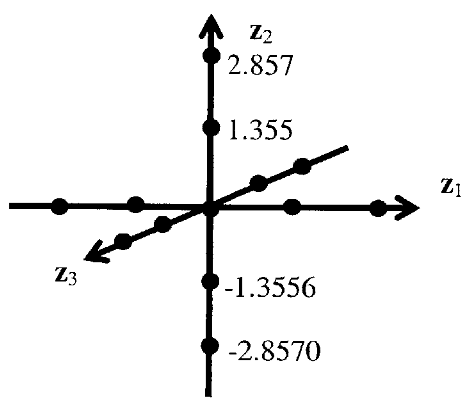


Figure 2.2 Sampling scheme for a system with three noise factors (n=3) and using the $4n$+1 rule.

If these variables are normally distributed with mean $\bar{z}_i$ and variance σ_i^2 , the corresponding design is $z_i = \bar{z}_i + \begin{pmatrix} -2.857 \\ 1.3556 \\ -1.3556 \\ 2.857 \end{pmatrix} \sigma_i$.

The quadrature-based method for multi-dimensional integration can be written:

$$Q[y] = y(\bar{z}) + \sum_{i=1}^{n} \sum_{j=1}^{N_i - 1} \alpha_i^{(j)} \left[y\left(D_i^{(j)} e_i + \bar{z}\right) - y(\bar{z}) \right] \quad (2.2)$$

where y is a polynomial function, n is the number of dimensions of the response function, N_i is the number of points used in the i^{th} dimension, $\bar{z}$ is the $n \times 1$ vector for means of variables, $\boldsymbol{\alpha}_i$ is the $(N_i - 1) \times 1$ vector for the Hermite-Gaussian quadrature weights in the i^{th} dimension, $\mathbf{D}_i$ is the $(N_i - 1) \times 1$ vector for the Hermite-Gaussian quadrature locations in the i^{th} dimension, $\alpha_i^{(j)}$ is the j^{th} element in the i^{th} weight vector and $D_i^{(j)}$ is the j^{th} element in the i^{th} location vector, e_i is the vector for dimension i: $e_i = [\delta_{1i} \quad \delta_{2i} \quad ,\cdots, \quad \delta_{ni}]^T$, and $\delta_{ij} = \begin{cases} 0 & if \quad i \neq j \\ 1 & if \quad i = j \end{cases}$.

Theorem 1

Suppose that we have a set of $(\boldsymbol{\alpha}_i, \mathbf{D}_i)$ such that $Q[y_i]$ is exact for a space of $y_i(z) \in Y_Q$, i.e.

$$\exists \ (\alpha_i, \ D_i) \qquad Q[y_i(z_i)] = E[y_i(z_i)] \qquad \forall \ i, \ y_i(z_i) \in Y_Q \quad (2.3)$$

Then $Q[y]$ is exact for any separable function

$$y(z) = y(\bar{z}) + \sum_{i=1}^{n} \hat{y}_i(z_i) \quad \text{where} \quad \hat{y}_i \in Y_Q \quad (2.4)$$

Proof:

For any separable function $y(z)$, we have

$$E[y] = y(\bar{z}) + \sum_{i=1}^{n} E[\hat{y}_i] \quad (2.5)$$

As shown in Equation 2.2, the mean of $y(z)$ can also be obtained using the Quadrature-based method

$$\begin{aligned} Q[y] &= y(\bar{z}) + \sum_{i=1}^{n} \sum_{j=1}^{N-1} \alpha^{(j)} \left[y\left(D_i^{(j)} e_i + \bar{z}\right) - y(\bar{z}) \right] \\ &= y(\bar{z}) + \sum_{i=1}^{n} \sum_{j=1}^{N-1} \alpha^{(j)} \left[\hat{y}_i\left(z^{(j)} e_i\right) \right] \\ &= y(\bar{z}) + \sum_{i=1}^{n} Q[\hat{y}_i] \\ &= y(\bar{z}) + \sum_{i=1}^{n} E[\hat{y}_i] = E[y] \end{aligned} \quad (2.6)$$

End of Theorem 1.

Under the assumption of separable function, theorem 1 proves that the exact mean of a multi-dimensional polynomial response function can be obtained using the quadrature-based method. However, the transmitted variance formula involves

$\left(y(z)-E\left[y(z)\right]\right)^2$ which seems to be an un-separable function even if $y(z)$ is separable. Nevereless, theorem 2 proves that the quadrature-based method can still provide the exact variance if $y(z)$ is a separable function shown in Equation 2.4 and $\hat{y}_i$ and $\hat{y}_j$ are independent $\forall \quad i \neq j$.

Theorem 2:

Assume that the response function $y(z)$ can be expressed as the sum of functions in single variables z_i

$$y(z) = y(\bar{z}) + \sum_{i=1}^{n} \hat{y}_i(z_i) \tag{2.7}$$

and $\hat{y}_i$ and $\hat{y}_j$ are independent $\forall \quad i \neq j$, then the variance of $y(z)$ is

$$\sigma_y^2 = \sum_{i=1}^{n} E\left[\hat{y}_i^2\right] - \left(E[\hat{y}_i]\right)^2 \tag{2.8}$$

Proof:
The mean of any separable function $y(z)$ is

$$E\left[y(z)\right] = y(\bar{z}) + \sum_{i=1}^{n} E[\hat{y}_i] \tag{2.9}$$

The variance of $y(z)$ is

$$\sigma_y^2 = E\left[y^2(z)\right] - \left(E\left[y(z)\right]\right)^2 \tag{2.10}$$

The first term of Equation 2.10 can be expressed as the function of expected values in single variables.

$$\begin{aligned} E\left[y^2\right] &= E\left[\left(y(\bar{z}) + \sum_{i=1}^{n} \hat{y}_i\right)^2\right] \\ &= \sum_{i=1}^{n} E\left[\hat{y}_i^2\right] + 2 \cdot y(\bar{z}) \cdot \sum_{i=1}^{n} E[\hat{y}_i] + y(\bar{z})^2 + 2\sum_{i=1}^{n} \sum_{\substack{j=1 \\ i<j}}^{n} E[\hat{y}_i] E\left[\hat{y}_j\right] \end{aligned} \tag{2.11}$$

Note that the last term in the second row of Equation 2.11 applied the assumption that $\hat{y}_i$ and $\hat{y}_j$ are independent.

Next, the last term in the Equation 2.10 is

$$\begin{aligned} \left(E\left[y(z)\right]\right)^2 &= \left(\sum_{i=1}^{n} E[\hat{y}_i] + y(\bar{z})\right)^2 \\ &= \left(\sum_{i=1}^{n} E[\hat{y}_i]\right)^2 + 2 \cdot y(\bar{z}) \cdot \sum_{i=1}^{n} E[\hat{y}_i] + y(\bar{z})^2 \end{aligned} \tag{2.12}$$

Substituting Equation 2.11 and Equation 2.12 into Equation 2.10, we can obtain the variance of the response function $y(z)$:

$$\begin{aligned}\sigma_y^2 &= \sum_{i=1}^{n} E\left[\hat{y}_i^2\right] - \left(\sum_{i=1}^{n} E[\hat{y}_i]\right)^2 + 2\sum_{i=1}^{n}\sum_{\substack{j=1 \\ i<j}}^{n} E[\hat{y}_i]E\left[\hat{y}_j\right] \\ &= \sum_{i=1}^{n} E\left[\hat{y}_i^2\right] - \sum_{i=1}^{n}\left(E[\hat{y}_i]\right)^2 = \sum_{i=1}^{n}\sigma_{\hat{y}_i}^2\end{aligned} \tag{2.13}$$

End of Theorem 2.

In 2004, Reber derived a transmitted variance formula different from Equation 2.13. Reber's thesis Equations 3.16 and 3.17, which together are a similar version of Equation 2.11 in this thesis, lack the term $2\sum_{i=1}^{n}\sum_{\substack{j=1 \\ i<j}}^{n} E[\hat{y}_i]E\left[\hat{y}_j\right]$ for calculating $E\left[y^2\right]$.

Reber stated that "No terms of the form $\hat{y}_i \cdot \hat{y}_j$ appear in Equation 3.17 because those terms would represent polynomials in two dimensions, and thus involve interactions... Including those terms would require us to use Cubature formula instead of Quadrature." In fact, as long as $\hat{y}_i$ and $\hat{y}_j$ are independent, the term $2\sum_{i=1}^{n}\sum_{\substack{j=1 \\ i<j}}^{n} E[\hat{y}_i]E\left[\hat{y}_j\right]$ can be estimated using the quadrature-based method. Thus, Reber's transmitted variance formula (Equation 3.22 in Reber's thesis P.36) is effectively equal to

$$\sigma_y^2 = \sum_{i=1}^{n} E\left[\hat{y}_i^2\right] - \sum_{i=1}^{n}\left(E[\hat{y}_i]\right)^2 - 2\sum_{i=1}^{n}\sum_{\substack{j=1 \\ i<j}}^{n} E[\hat{y}_i]E\left[\hat{y}_j\right] \tag{2.14}$$

Comparing Reber's transmitted variance formula (Equation 2.14) with Equation 2.13, we find that Reber's transmitted variance formula will report a transmitted variance different to the result reported by Equation 2.13. Let's take a separable function $y(z_1, z_2) = z_1^2 + z_2^2$ as an example, where z_1 and z_2 are independent standard normally distributed random variables. It is obvious that the expected value of y is 2 and the variance σ_y^2 is 4. However, Reber's transmitted variance formula reports 2. Thus, Reber's formula gives a 50% error in estimating the transmitted variance in this case. The updated transmitted variance formula (Equation 2.13) in Theorem 1 gives the exact right answer, σ_y^2=4.

Theorem 2 proves that, if the response function is separable and independent, the total transmitted variance is the summation of variance in each dimension. Therefore, if we can find a set of $(\alpha_i, \mathbf{D}_i)$ such that $Q\left[y_i^2\right]$ is exact for a space of $y_i^2(z) \in Y_Q^2$,

i.e. $\exists \ (\alpha_i, \ D_i) \quad Q\left[y_i^2(z_i)\right] = E\left[y_i^2(z_i)\right] \quad \forall \ i, y_i^2(z_i) \in Y_Q^2$, then the variance of the response function obtained using the quadrature-based method is exact.

For simulated engineering systems from hierarchical probability models in Chapter 4 and case studies in Chapter 5, the five-point quadrature-based method is used to study its accuracy in estimating the output mean and transmitted variance. From theorem 1 and 2, we know that the five point quadrature-based method can give the exact output mean for separable polynomial function up to 9^{th} order and the exact transmitted variance for separable polynomial function up to 4^{th} order. It is still necessary here to analyze the accuracy of the five-point quadrature-based method in estimating the output mean and the transmitted variance when responses are higher-order separable polynomial functions.

The mean of a n-variable response function is defined as

$$E\left[y(z)\right] \equiv \int_{-\infty}^{+\infty} \ldots \int_{-\infty}^{+\infty} w(z)\, y(z)\, dz \tag{2.15}$$

where $w(z)$ is the probability density function of $y(z)$. If the response function is continuous, differentiable at $\overline{z}$, and also separable, the k-th order Taylor series approximation of $y(z)$ at $y(\overline{z})$ is

$$y(z) = y(\overline{z}) + \sum_{j=1}^{k} \frac{1}{j!} \sum_{i=1}^{n} \left(\hat{z}_i \frac{\partial}{\partial \hat{z}_i} \right)^j y + R_{k+1} \tag{2.16}$$

where $\hat{z}_i = z_i - \overline{z}_i$,

$$R_{k+1} = \frac{1}{(k+1)!} \sum_{i=1}^{n} \left(\hat{z}_i \frac{\partial}{\partial \hat{z}_i} \right)^{k+1} y(z_1^0 + \theta \hat{z}_1, z_2^0 + \theta \hat{z}_2, \ldots, z_n^0 + \theta \hat{z}_n) \tag{2.17}$$

and $0 < \theta < 1$.

Using the Taylor series approximation of $y(z)$ at $y(\bar{z})$, we can obtain the mean of $y(z)$ by both the direct integration and the quadrature-based method.

$$E\left[y(z)\right]_{Exact} = y(\bar{z})+\sum_{i=1}^{n}\left(\frac{1}{2!}\frac{\partial^2 y}{\partial\hat{z}_i^2}\sigma_i^2+\frac{3}{4!}\frac{\partial^4 y}{\partial\hat{z}_i^4}\sigma_i^4+\frac{15}{6!}\frac{\partial^6 y}{\partial\hat{z}_i^6}\sigma_i^6+\frac{105}{8!}\frac{\partial^8 y}{\partial\hat{z}_i^8}\sigma_i^8+\frac{945}{10!}\frac{\partial^{10} y}{\partial\hat{z}_i^{10}}\sigma_i^{10}\ldots\right) \quad (2.18)$$

$$Q\left[y(z)\right] = y(\bar{z})+\sum_{i=1}^{n}\left(\frac{1}{2!}\frac{\partial^2 y}{\partial\hat{z}_i^2}\sigma_i^2+\frac{3}{4!}\frac{\partial^4 y}{\partial\hat{z}_i^4}\sigma_i^4+\frac{15}{6!}\frac{\partial^6 y}{\partial\hat{z}_i^6}\sigma_i^6+\frac{105}{8!}\frac{\partial^8 y}{\partial\hat{z}_i^8}\sigma_i^8+\frac{825}{10!}\frac{\partial^{10} y}{\partial\hat{z}_i^{10}}\sigma_i^{10}\ldots\right) \quad (2.19)$$

The relative error mean is obtained by subtracting Equation 2.18 from Equation 2.19 and then divided by Equation 2.19.

$$\varepsilon_\mu = \frac{\sum_{i=1}^{n}\left(\frac{120}{10!}\frac{\partial^{10} y}{\partial\hat{z}_i^{10}}\sigma_i^{10}\ldots\right)}{y(\bar{z})+\sum_{i=1}^{n}\left(\frac{1}{2!}\frac{\partial^2 y}{\partial\hat{z}_i^2}\sigma_i^2+\frac{3}{4!}\frac{\partial^4 y}{\partial\hat{z}_i^4}\sigma_i^4+\frac{15}{6!}\frac{\partial^6 y}{\partial\hat{z}_i^6}\sigma_i^6+\frac{105}{8!}\frac{\partial^8 y}{\partial\hat{z}_i^8}\sigma_i^8+\frac{945}{10!}\frac{\partial^{10} y}{\partial\hat{z}_i^{10}}\sigma_i^{10}\ldots\right)} \quad (2.20)$$

The five-point quadrature-based method can estimate the output mean exactly when the separable response is a polynomial function up to ninth order. If the response has a tenth order polynomial term, the coefficient of σ_i^{10} in the numerator is typically very small. And it is also very likely that the term $y(\bar{z})$ is the dominating terms in practical engineering systems. Hence, the quadrature-based method is likely to give very accurate result in estimating the output mean for tenth-order separable polynomial systems.

Similarly, the transmitted variance of any separable function can be obtained by both the direct integration and the five-point quadrature-based method (Equation 2.21 and 2.22)

$$\sigma_{Exact}^2=\sum_{i=1}^{n}\left(\begin{array}{l}\left(\frac{\partial y}{\partial\hat{z}_i}\right)^2\sigma_i^2+\left[\frac{1}{2}\left(\frac{\partial^2 y}{\partial\hat{z}_i^2}\right)^2+\frac{\partial y}{\partial\hat{z}_i}\frac{\partial^3 y}{\partial\hat{z}_i^3}\right]\sigma_i^4\\+\left[15\left(\frac{1}{3!}\frac{\partial^3 y}{\partial\hat{z}_i^3}\right)^2+\frac{30}{5!}\left(\frac{\partial y}{\partial\hat{z}_i}\frac{\partial^5 y}{\partial\hat{z}_i^5}\right)+\frac{1}{2}\left(\frac{\partial^2 y}{\partial\hat{z}_i^2}\frac{\partial^4 y}{\partial\hat{z}_i^4}\right)\right]\sigma_i^6\\+\left[\frac{96}{4!4!}\left(\frac{\partial^4 y}{\partial\hat{z}_i^4}\right)^2+\frac{210}{7!}\left(\frac{\partial y}{\partial\hat{z}_i}\frac{\partial^7 y}{\partial\hat{z}_i^7}\right)+\frac{90}{6!}\left(\frac{\partial^2 y}{\partial\hat{z}_i^2}\frac{\partial^6 y}{\partial\hat{z}_i^6}\right)+\frac{210}{3!5!}\left(\frac{\partial^3 y}{\partial\hat{z}_i^3}\frac{\partial^5 y}{\partial\hat{z}_i^5}\right)\right]\sigma_i^8\\+\left[\begin{array}{l}\frac{945}{5!5!}\left(\frac{\partial^5 y}{\partial\hat{z}_i^5}\right)^2+\frac{2\times 945}{1!9!}\left(\frac{\partial y}{\partial\hat{z}_i}\frac{\partial^9 y}{\partial\hat{z}_i^9}\right)+\frac{2\times 840}{2!8!}\left(\frac{\partial^2 y}{\partial\hat{z}_i^2}\frac{\partial^8 y}{\partial\hat{z}_i^8}\right)\\+\frac{2\times 945}{3!7!}\left(\frac{\partial^3 y}{\partial\hat{z}_i^3}\frac{\partial^7 y}{\partial\hat{z}_i^7}\right)+\frac{2\times 840}{4!6!}\left(\frac{\partial^4 y}{\partial\hat{z}_i^4}\frac{\partial^6 y}{\partial\hat{z}_i^6}\right)\end{array}\right]\sigma_i^{10}+\cdots\end{array}\right) \qquad (2.21)$$

$$\sigma_Q^2=\sum_{i=1}^{n}\left(\begin{array}{l}\left(\frac{\partial y}{\partial\hat{z}_i}\right)^2\sigma_i^2+\left[\frac{1}{2}\left(\frac{\partial^2 y}{\partial\hat{z}_i^2}\right)^2+\frac{\partial y}{\partial\hat{z}_i}\frac{\partial^3 y}{\partial\hat{z}_i^3}\right]\sigma_i^4\\+\left[\frac{5}{12}\left(\frac{\partial^3 y}{\partial\hat{z}_i^3}\right)^2+\frac{30}{5!}\frac{\partial y}{\partial\hat{z}_i}\frac{\partial^5 y}{\partial\hat{z}_i^5}+\frac{1}{2}\frac{\partial^2 y}{\partial\hat{z}_i^2}\frac{\partial^4 y}{\partial\hat{z}_i^4}\right]\sigma_i^6\\+\left[\frac{96}{4!4!}\left(\frac{\partial^4 y}{\partial\hat{z}_i^4}\right)^2+\frac{220}{7!}\frac{\partial y}{\partial\hat{z}_i}\frac{\partial^7 y}{\partial\hat{z}_i^7}+\frac{90}{6!}\frac{\partial^2 y}{\partial\hat{z}_i^2}\frac{\partial^6 y}{\partial\hat{z}_i^6}+\frac{210}{3!5!}\frac{\partial^3 y}{\partial\hat{z}_i^3}\frac{\partial^5 y}{\partial\hat{z}_i^5}\right]\sigma_i^8\\+\left[\begin{array}{l}\frac{825}{5!5!}\left(\frac{\partial^5 y}{\partial\hat{z}_i^5}\right)^2+\frac{2\times 825}{1!9!}\left(\frac{\partial y}{\partial\hat{z}_i}\frac{\partial^9 y}{\partial\hat{z}_i^9}\right)+\frac{2\times 825}{2!8!}\left(\frac{\partial^2 y}{\partial\hat{z}_i^2}\frac{\partial^8 y}{\partial\hat{z}_i^8}\right)\\+\frac{2\times 825}{3!7!}\left(\frac{\partial^3 y}{\partial\hat{z}_i^3}\frac{\partial^7 y}{\partial\hat{z}_i^7}\right)+\frac{2\times 825}{4!6!}\left(\frac{\partial^4 y}{\partial\hat{z}_i^4}\frac{\partial^6 y}{\partial\hat{z}_i^6}\right)\end{array}\right]\sigma_i^{10}+\ldots\end{array}\right) \qquad (2.22)$$

Using the following notations, $\beta_0=y(\bar{z})$, $\beta_i=\frac{\partial y}{\partial\hat{z}_i}\sigma_i$, $\beta_{ii}=\frac{1}{2!}\frac{\partial^2 y}{\partial\hat{z}_i^2}\sigma_i^2$, $\beta_{iii}=\frac{1}{3!}\frac{\partial^3 y}{\partial\hat{z}_i^3}\sigma_i^3$, $\beta_{iiii}=\frac{1}{4!}\frac{\partial^4 y}{\partial\hat{z}_i^4}\sigma_i^4$, and $\beta_{iiiii}=\frac{1}{5!}\frac{\partial^5 y}{\partial\hat{z}_i^5}\sigma_i^5$, the relative error variance of fifth-order separable polynomial functions can be obtained by subtracting the Equation 2.22 from the exact variance (Equation 2.21) and then divided by exact variance (Equation 2.21).

$$\varepsilon_{\sigma^2}=\frac{\sum_{i=1}^{n}-120\beta_{iiiii}^{\ 2}}{\sum_{i=1}^{n}\beta_i^2+2\beta_{ii}^{\ 2}+6\beta_i\beta_{iii}+15\beta_{iii}^{\ 2}+24\beta_{ii}\beta_{iiii}+96\beta_{iiii}^{\ 2}+30\beta_i\beta_{iiiii}+210\beta_{iii}\beta_{iiiii}+945\beta_{iiiii}^{\ 2}} \qquad (2.23)$$

The five-point quadrature-based method can estimate the transmitted variance exactly when the separable response is a polynomial function up to fourth order. For fifth-order polynomial functions, the relative error variance is smaller than zero. The denominator of the relative error variance (Equation 2.23) comes from the exact variance (Equation 2.21). Thus the denominator must be a positive number. The numerator is smaller than zero. Then, the relative error variance is smaller than zero. Therefore, the five-point quadrature-based method is biased in estimating the transmitted variance of fifth-order separable polynomial functions. For six or higher-order polynomial functions, the relative error variance could be positive or negative.

Chapter 3

The Comparison between the Quadrature-based Method and the Sensitivity-based Method

The sensitivity-based method [e.g., first-order first-moment (FOFM), first-order second-moment (FOSM), second-order first-moment (SOFM), and second-order second-moment (SOSM)] has been widely used in product development to estimate the output mean and variance of a response function $y(z)$ (e.g., Solari et al. 2001; Malkawi et al. 2000; Huang et al. 2005). As introduced in chapter 1, this method starts from approximating the response function $y(z)$ by a low-order Taylor series and computes the mean and variance from the approximated function. The error in estimating the output mean and variance comes from the truncation error in approximating the response function $y(z)$ and the numerical error in estimating the derivatives of $y(z)$. The calculation of derivatives of $y(z)$ may involve significant computational effort. Despite this, the sensitivity-based method is still widely used in early product development.

This chapter compares the Quadrature-based method and sensitivity-based method and makes suggestions to practitioners to improve the accuracy of the sensitivity-based method.

We start with comparing the Quadrature-based method and sensitivity-based method in single variable case. The conclusion can be extended to multi-dimensional separable function.

For the sensitivity-based method, the mean of the single variable response function $y(z)$ can be approximated by SOFM

$$E\left[y(z)\right]_{SOFM} = y(\bar{z}) + \frac{1}{2!}\frac{\partial^2 y}{\partial \hat{z}^2}\sigma^2 \tag{3.1}$$

The variance of the response function $y(z)$ approximated by SOSM is

$$\sigma_{SOSM}^2 = \left(\frac{\partial y}{\partial \hat{z}}\right)^2 \sigma^2 + \frac{1}{2}\left(\frac{\partial^2 y}{\partial \hat{z}^2}\right)^2 \sigma^4 \tag{3.2}$$

where in practice the derivatives usually are

$$\frac{\partial y}{\partial \hat{z}} \approx \frac{y(\Delta\hat{z}) - y(-\Delta\hat{z})}{2\times\Delta\hat{z}}, \quad \frac{\partial^2 y}{\partial \hat{z}^2} \approx \frac{y(\bar{z}+\Delta\hat{z}) - 2y(\bar{z}) + y(\bar{z}-\Delta\hat{z})}{\Delta\hat{z}^2}, \tag{3.3}$$

and $\Delta\hat{z} = (0.01 \sim 0.05)\bar{z}$.

The errors of SOFM and SOSM of $y(z)$ come from truncation errors in Taylor approximation and numerical errors in estimating derivatives. The Quadrature-based method is typically more accurate than SOFM and SOSM because the truncation error in the Quadrature-based method is usually smaller than the truncation error in the SOFM and SOSM.

Further consideration shows that if $\Delta\hat{z} = 1.732\sigma$ is used to calculate the derivatives that are used in the sensitivity-based method, the SOFM and SOSM could give the same result as the three-point Quadrature-based method. The details are illustrated in Equations 3.4 to 3.7 by simply letting $\Delta\hat{z} = 1.732\sigma$.

Letting $\Delta\hat{z} = 1.732\sigma$, we can derive the mean of the output using SOFM as

$$
\begin{aligned}
E\left[y(z)\right]_{SOFM} &= y(\bar{z}) + \frac{1}{2!}\frac{\partial^2 y}{\partial \hat{z}^2}\sigma^2 \\
&= y(\bar{z}) + \frac{1}{2!}\frac{y(\bar{z}+\Delta\hat{z}) - 2y(\bar{z}) + y(\bar{z}-\Delta\hat{z})}{\Delta\hat{z}^2}\sigma^2 \\
&= y(\bar{z}) + \frac{1}{2!}\frac{y(\bar{z}+1.732\sigma) - 2y(\bar{z}) + y(\bar{z}-1.732\sigma)}{(1.732\sigma)^2}\sigma^2 \\
&= \frac{2}{3}y(\bar{z}) + \frac{1}{6}y(\bar{z}+1.732\sigma) + \frac{1}{6}y(\bar{z}-1.732\sigma)
\end{aligned}
\tag{3.4}
$$

The three-point Quadrature-based method for estimating the mean $E\left[y(z)\right]$ is

$$
\begin{aligned}
Q[y] &= y(\bar{z}) + \sum_{j=1}^{2}\alpha^{(j)}\left[y(z^{(j)}) - y(\bar{z})\right] \\
&= y(\bar{z}) + \frac{1}{6}\left[y(\bar{z}+1.732\sigma) - y(\bar{z})\right] + \frac{1}{6}\left[y(\bar{z}-1.732\sigma) - y(\bar{z})\right] \\
&= \frac{2}{3}y(\bar{z}) + \frac{1}{6}y(\bar{z}+1.732\sigma) + \frac{1}{6}y(\bar{z}-1.732\sigma)
\end{aligned}
\tag{3.5}
$$

Obviously, Equation 3.4 and 3.5 give the same mean of the output.

Letting $\Delta\hat{z} = 1.732\sigma$, we can derive the variance using SOSM as

$$
\begin{aligned}
\sigma_{SOSM}^2 &= \left(\frac{\partial y}{\partial \hat{z}}\right)^2\sigma^2 + \frac{1}{2}\left(\frac{\partial^2 y}{\partial \hat{z}^2}\right)^2\sigma^4 \\
&= \left(\frac{y(\bar{z}+\Delta\hat{z}) - y(\bar{z}-\Delta\hat{z})}{2\Delta\hat{z}}\right)^2\sigma^2 + \frac{1}{2}\left(\frac{y(\bar{z}+\Delta\hat{z}) - 2y(\bar{z}) + y(\bar{z}-\Delta\hat{z})}{\Delta\hat{z}^2}\right)^2\sigma^4 \\
&= \left(\frac{y(\bar{z}+1.732\sigma) - y(\bar{z}-1.732\sigma)}{2\times 1.732\sigma}\right)^2\sigma^2 + \frac{1}{2}\left(\frac{y(\bar{z}+1.732\sigma) - 2y(\bar{z}) + y(\bar{z}-1.732\sigma)}{(1.732\sigma)^2}\right)^2\sigma^4 \\
&= \frac{2}{9}y^2(\bar{z}) + \frac{5}{36}y^2(\bar{z}+1.732\sigma) + \frac{5}{36}y^2(\bar{z}-1.732\sigma) - \frac{1}{18}y(\bar{z}+1.732\sigma)\times y(\bar{z}-1.732\sigma) \\
&\quad - \frac{2}{9}y(\bar{z}+1.732\sigma)\times y(\bar{z}) - \frac{2}{9}y(\bar{z})\times y(\bar{z}-1.732\sigma)
\end{aligned}
\tag{3.6}
$$

The three-point Quadrature-based method for estimating the variance is

$$
\begin{aligned}
\sigma_{Q\_3Points}^2 &= Q\left[(y)^2\right] - (Q[y])^2 \\
&= \frac{2}{3}y^2(\bar{z}) + \frac{1}{6}y^2(\bar{z}+1.732\sigma) + \frac{1}{6}y^2(\bar{z}-1.732\sigma) \\
&\quad - \left(\frac{2}{3}y(\bar{z}) + \frac{1}{6}y(\bar{z}+1.732\sigma) + \frac{1}{6}y(\bar{z}-1.732\sigma)\right)^2 \\
&= \frac{2}{9}y^2(\bar{z}) + \frac{5}{36}y^2(\bar{z}+1.732\sigma) + \frac{5}{36}y^2(\bar{z}-1.732\sigma) - \frac{1}{18}y(\bar{z}+1.732\sigma)\times y(\bar{z}-1.732\sigma) \\
&\quad - \frac{2}{9}y(\bar{z}+1.732\sigma)\times y(\bar{z}) - \frac{2}{9}y(\bar{z})\times y(\bar{z}-1.732\sigma)
\end{aligned}
\tag{3.7}
$$

Equation 3.6 and 3.7 give the same result. Thus, the SOFM and SOSM could give the same result as the three-point Quadrature-based method when $\Delta\hat{z}$ is equal to 1.732σ. Further improvement of sensitivity based method is possible by using the same five-points of the Qudrature-based method. This conclusion can be extended to multi-dimension separable response functions based on the analysis in Chapter 2.

The purpose of using Hermite-Gassian quadrature points to calculate the derivatives in the sensitivity-based method is not to reduce the numerical error in the calculation of derivatives. Instead, it reduces the error due to the approximation of the response function $y(z)$ using a low-order Taylor series.

Thus, the Quadrature-based method provides a simple, direct, and accurate method to calculate the mean and variance of separable response function $y(z)$. Adopting the Quadrature-based method may have a big impact on practitioners in early stages of product development.

Chapter 4

Model-based Evaluation for Un-Separable Polynomial Systems

The proposed method described in chapter 2 has been proven to have very good accuracy for separable polynomial systems. The method gives exact transmitted variance if the response is up to a fourth-order separable polynomial and less than 5% error of transmitted variance for a fifth-order separable polynomial. These separable polynomial systems assume that only single factor effects exist. As we know, in most engineering applications, the interaction effects cannot be ignored and they should be included in the polynomial models. This chapter starts the investigation of the accuracy of the quadrature-based method in the face of un-separable, polynomial systems that include interaction effects.

4.1 The Third-Order Un-Separable Polynomial Model-based Evaluation

For un-separable polynomial response systems, the accuracy of the quadrature-based 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. It has long been observed in Design of Experiments that higher-order interactions among factors are relatively less frequent than main effects. This effect hierarchy principle is a relatively stable regularity and has been used to good effect in engineering practice. The hierarchical probability model was proposed by Chipman, Wu, and Hamada (1997) as a means to more effectively derive polynomial response models from experiments with complex aliasing patterns. This model was fit to data from 113 full factorial engineering experiments by Li and Frey (2005). The fitted model is useful for evaluating various techniques for robust design with computer experiments. Equations 4.1 through 4.8 comprise the model used here.

$$y = \sum_{i=1}^{n} \beta_i z_i + \sum_{j=1}^{n} \sum_{\substack{i=1 \\ i \le j}}^{n} \beta_{ij} z_i z_j + \sum_{k=1}^{n} \sum_{\substack{j=1 \\ j \le k}}^{n} \sum_{\substack{i=1 \\ i \le j}}^{n} \beta_{ijk} z_i z_j z_k \tag{4.1}$$

$$z_i \sim N(0, \varepsilon^2), \text{ where } \varepsilon = 10\% \tag{4.2}$$

$$f(\beta_i | \delta_i) = \begin{cases} N(0,1) & \text{if } \delta_i = 0 \\ N(0,10^2) & \text{if } \delta_i = 1 \end{cases} \tag{4.3}$$

$$f(\beta_{ij} | \delta_{ij}) = \begin{cases} N(0,1) & \text{if } \delta_{ij} = 0 \\ N(0,10^2) & \text{if } \delta_{ij} = 1 \end{cases} \tag{4.4}$$

$$f(\beta_{ijk} | \delta_{ijk}) = \begin{cases} N(0,1) & \text{if } \delta_{ijk} = 0 \\ N(0,10^2) & \text{if } \delta_{ijk} = 1 \end{cases} \tag{4.5}$$

$$\Pr(\delta_i = 1) = p \tag{4.6}$$

$$\Pr(\delta_{ij} = 1 | \delta_i, \delta_j) = \begin{cases} p_{00} & \text{if } \delta_i + \delta_j = 0 \\ p_{01} & \text{if } \delta_i + \delta_j = 1 \\ p_{11} & \text{if } \delta_i + \delta_j = 2 \end{cases} \tag{4.7}$$

$$\Pr(\delta_{ijk} = 1 | \delta_i, \delta_j, \delta_k) = \begin{cases} p_{000} & \text{if } \delta_i + \delta_j + \delta_k = 0 \\ p_{001} & \text{if } \delta_i + \delta_j + \delta_k = 1 \\ p_{011} & \text{if } \delta_i + \delta_j + \delta_k = 2 \\ p_{111} & \text{if } \delta_i + \delta_j + \delta_k = 3 \end{cases} \tag{4.8}$$

Equation 4.1 expresses the assumption that the system response is a third-order polynomial. Equation 4.2 defines the input variations as random normal variables. We use a standard deviation of 10% because it represents a level of difficulty for the methods comparable to that found in most case studies we find in the literature. Equations 4.3 through 4.5 assign probability distributions to the polynomial coefficients. Polynomial coefficients β_i whose corresponding parameters $\delta_i = 1$ have a larger probability of taking on a large positive or negative value. The values of the parameters δ_i are set in Equations 4.6 through 4.8. The values of the parameters in the model are taken from an empirical study of 113 full factorial experiments (Li and Frey 2005) 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 are sampled from the probability model (Equations 4.1 through 4.8). The expected value and transmitted variance of the response y are estimated in six ways:

1) using the Hermite-Gaussian quadrature technique which requireds $4n+1$ samples
2) generating $4n+1$ samples via LHS and computing their mean and variance
3) generating $4n+1$ samples via HSS and computing their mean and variance
4) generating $10\times(4n+1)$ samples via LHS and computing their mean and variance
5) generating $10\times(4n+1)$ samples via HSS and computing their mean and variance
6) generating n^2+3n+3 samples via Lu and Darmofal (2005)'s cubature method and computing their mean and variance.

Since the noise factors are standard, normally distributed, independent random variables, the expected value of the response function $y(z)$ can be determined by direct integration

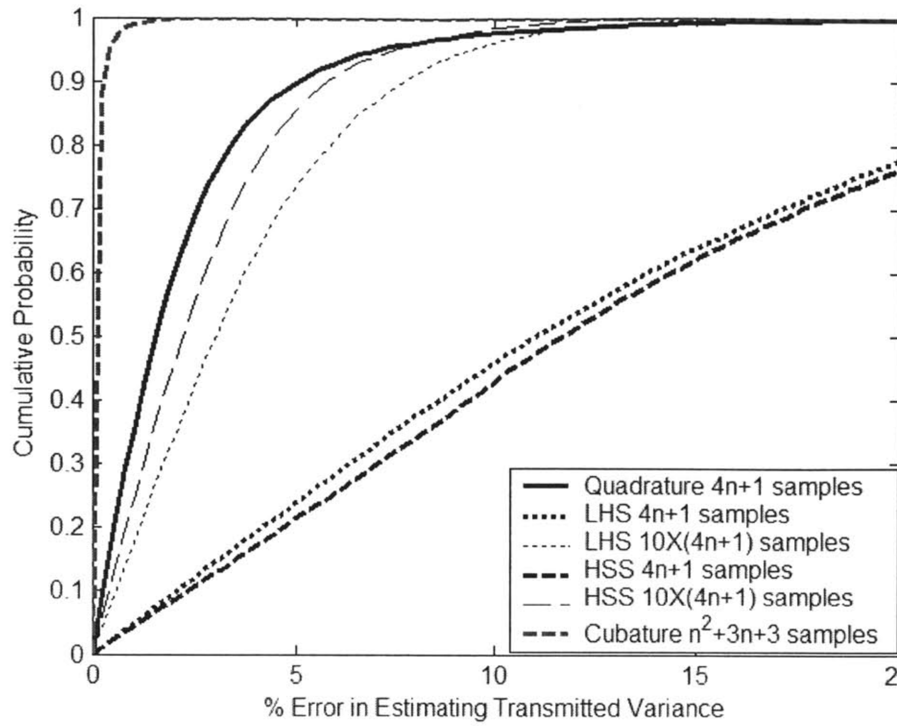
$$E[y(z)] = \sum_{j=1}^{n}\sum_{\substack{i=1 \\ i\le j}}^{n} \varepsilon^2 \beta_{ij} \tag{4.9}$$

Similarly, the closed form solution of the transmitted variance, $\sigma^2_{Exact} = E[y^2] - (E[y])^2$, can also be determined by direct integration of y and y^2. The result is simplified in Equation 4.10.

$$\begin{aligned}
\sigma^2_{Exact}\left(y(z)\right) &= \sum_{i=1}^{n}\left(\varepsilon^2\beta_i^{\,2} + 2\varepsilon^4\beta_{ii}^{\,2} + 6\varepsilon^4\beta_i\beta_{iii} + 15\varepsilon^6\beta_{iii}^{\,2}\right) \\
&+ \sum_{i=1}^{n}\sum_{\substack{j=1 \\ i\le j}}^{n}\begin{pmatrix} \varepsilon^4\beta_{ij}^{\,2} + 3\varepsilon^6\beta_{iij}^{\,2} + 3\varepsilon^6\beta_{ijj}^{\,2} + 2\varepsilon^4\beta_i\beta_{ijj} \\ +2\varepsilon^4\beta_j\beta_{iij} + 6\varepsilon^6\beta_{iii}\beta_{ijj} + 6\varepsilon^6\beta_{jjj}\beta_{iij} \end{pmatrix} \\
&+ \sum_{i=1}^{n}\sum_{\substack{j=1 \\ i\le j}}^{n}\sum_{\substack{k=1 \\ j\le k}}^{n}\varepsilon^6\left(\beta_{ijk}^{\,2} + 2\beta_{iij}\beta_{jkk} + 2\beta_{iik}\beta_{jjk} + 2\beta_{ijj}\beta_{ikk}\right)
\end{aligned} \tag{4.10}$$

Equations 4.9 and 4.10 enable the computation of the size of the error for each of the 15,000 systems given each of the six ways. These data are used to estimate the cumulative probability versus error (Figure 4.1). 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 4.1 shows that the quadrature technique estimates the transmitted varaince within 5% for more than 90% of all systems sampled. Quadrature accomplishes this with only $4n+1$ samples. HSS and LHS are unable to provide comparably good results with $4n+1$ samples. However, given ten times the resources, HSS achieves accuracy comparable to that of quadrature. Lu and Darmofal (2005)'s cubature method shows a very higher level of accuracy at the cost of n^2+3n+3 samples. For higher-dimension problems, practitioners may not be able to afford the samples required to run the Lu and Darmofal's cubature method. Hence the Hermite-Gaussian quadrature method provides an alternative tool for practitioners in the face of limited resources and time constraints.



# of Input factors	# of systems
6	1000
7	1000
8	1000
9	1000
10	1000
11	1000
12	1000
13	1000
14	1000
15	1000
16	1000
17	1000
18	1000
19	1000
20	1000
Total	15000

Figure 4.1 Cumulative probability versus error in estimating transmitted variance for six different sampling procedures. The Result is based on 15,000 systems generated from the Hierarchical Probability Model (Equations 4.1 to 4.8).

Based on the Hierarchical Probability Model, the cubature method shows a much higher level of accuracy than any other method. However, case studies in the next chapter illustrate that Lu and Darmofal's Cubature and the quadrature-based method have similar levels of accuracy. Thus, a further calibration of parameters might be needed to fit the Hierarchical Probability Model (Equations 4.1 to 4.8) to reality. However, we do not want to change the parameters from a published empirical study of 113 full factorial experiments. (Li and Frey 2005)

Furthermore, real engineering applications might need an evaluation of a higher-order polynomial response. Although Li and Frey were able to specify the parameters in the third-order probability model, based on the analysis of 113 full factorial engineering experiments, it is almost impossible to specify all parameters for the fourth, fifth, or higher-order polynomial response model because of the limited available full factorial engineering experiments and the numerous parameters in the higher-order models. Recently, Joseph (2006) published a probability model which can be used for higher-order polynomials with a much smaller number of parameters needing specification. In the next section, a comparison of the accuracy of the quadrature-based method and alternatives is made based on the extension of Joseph's probability model to account for the interaction terms.

4.2 Higher-Order Un-Separable Polynomial Model-based Evaluation

Joseph (2006) proposed a probability model based on the effect hierarchy principles. This model can be easily used to derive higher-order, separable multi-variable, polynomial response systems. Joseph assumed that the coefficients will be normally distributed with zero mean and the variance of the coefficients will reduce geometrically with the order of the terms. In this section Joseph's probability model is extended to investigate the accuracy of the quadrature-based method and other alternative sampling methods in un-separable, multi-variable response systems. A representative fifth-order un-separable, multi-variable polynomial response model is studied.

We compare the quadrature-based method presented and analyzed in previous chapters to some other methods. Again, the alternatives to be considered are Latin Hypercube Sampling (McKay et al., 1979), Hammersley Sequence Sampling (Diwekar, 1997), and Lu and Darmofal's cubature method (2005). All these methods are applied to 5,000 fifth-order, un-separable, polynomial response systems which are defined as

$$\begin{aligned} y(\mathbf{z}) = \beta_0 + \sum_{i=1}^{n}\beta_i\mathbf{z}_i + \sum_{j=1}^{n}\sum_{\substack{i=1\\ i\le j}}^{n}\beta_{ij}\mathbf{z}_i\mathbf{z}_j + \sum_{k=1}^{n}\sum_{\substack{j=1\\ j\le k}}^{n}\sum_{\substack{i=1\\ i\le j}}^{n}\beta_{ijk}\mathbf{z}_i\mathbf{z}_j\mathbf{z}_k + \\ \sum_{l=1}^{n}\sum_{\substack{k=1\\ k\le l}}^{n}\sum_{\substack{j=1\\ j\le k}}^{n}\sum_{\substack{i=1\\ i\le j}}^{n}\beta_{ijkl}\mathbf{z}_i\mathbf{z}_j\mathbf{z}_k\mathbf{z}_l + \sum_{m=1}^{n}\sum_{\substack{l=1\\ l\le m}}^{n}\sum_{\substack{k=1\\ k\le l}}^{n}\sum_{\substack{j=1\\ j\le k}}^{n}\sum_{\substack{i=1\\ i\le j}}^{n}\beta_{ijklm}\mathbf{z}_i\mathbf{z}_j\mathbf{z}_k\mathbf{z}_l\mathbf{z}_m \end{aligned} \tag{4.11}$$

where the independent variables are normally distributed random variables and the polynomial coefficients are also normally distributed and subject to geometric decay with increasing order.

$$\beta_i \sim N(0,\tau^2 r) \tag{4.12}$$

$$f(\beta_{ij}) = \begin{cases} N(0,\tau^2 r^2) & if \quad i=j \\ N(0,\tau^2 r_{INT}^2) & otherwise \end{cases} \tag{4.13}$$

$$f(\beta_{ijk}) = \begin{cases} N(0,\tau^2 r^3) & if \quad i=j=k \\ N(0,\tau^2 r_{INT}^3) & otherwise \end{cases} \tag{4.14}$$

$$f(\beta_{ijkl}) = \begin{cases} N(0,\tau^2 r^4) & if \quad i=j=k=l \\ N(0,\tau^2 r_{INT}^4) & otherwise \end{cases} \tag{4.15}$$

$$f(\beta_{ijklm}) = \begin{cases} N(0,\tau^2 r^5) & if \quad i=j=k=l=m \\ N(0,\tau^2 r_{INT}^5) & otherwise \end{cases} \tag{4.16}$$

It was shown empirically by Li and Frey (2005) via a meta-analysis of published experiments that second order effects are about 0.2 the size of first order effects on average across large populations of factorial experiments. This might suggest that $\sqrt{r}=0.2$. Thus, r =0.04 is a reasonable mean value for a prior probability of r. We set $\sqrt{r_{INT}/r}=0.6$ to represent a faster decay rate of two-factor interactions than second order single factor effects. Equations 4.12 to 4.16 imply the effect hierarchy principle. For r =0.04, the variance of a lower-order effect is larger than that of a higher-order effect. Hence the lower-order effect is more likely to be of larger magnitude and thus more important than a higher-order effect.

For each integer $n \in [4,8]$, one thousand systems were sampled from the probability model (Equations 4.11 through 4.16). The mean and variance of every response function y are estimated in six ways:

1) using the Hermite-Gaussian quadrature technique which requires $4n+1$ samples
2) generating $4n+1$ samples via LHS and computing their mean and variance
3) generating $4n+1$ samples via HSS and computing their mean and variance
4) generating $10\times(4n+1)$ samples via LHS and computing their mean and variance
5) generating $10\times(4n+1)$ samples via HSS and computing their mean and variance
6) generating n^2+3n+3 samples via Lu and Darmofal's Cubature method and computing their mean and variance.

This probability model is applied to dimension n that is smaller than or equal to eight. This is because of the computational difficulty in evaluating the huge number of terms in the fifth-order, polynomial response function (Equation 4.11). The number of calculation needed in evaluating Equation 4.11 is in the order of n^5 which increases very quickly when n is larger than eight.

Since the noise factors are standard, normally distributed, independent random variables, the expected value of the response function $y(z)$ can be determined by direct integration

$$E(y(\mathbf{z})) = \beta_0 + \sum_{i=1}^{n} \beta_{ii} + \sum_{i=1}^{n} 3\beta_{iiii} + \sum_{i=1}^{n} \sum_{\substack{j=1 \\ i<j}}^{n} \beta_{iijj} \tag{4.17}$$

The second term in Equation 4.17 captures the second-order single factor effects and the third term in Equation 4.17 captures the fourth-order interaction effects. Both third term and fourth terms cannot be captured in a third-order probability model. See Equation 4.9.

Similarly, the closed form solution of the transmitted variance, $\sigma^2_{Exact} = E[y^2] - (E[y])^2$, can also be determined by direct integration of y and y^2. The result is simplified in Equation 4.18.

$$
\begin{aligned}
\sigma^2(y(\mathbf{z})) = {} & \sum_{i=1}^{n}\left(\beta_i^2 + 2\beta_{ii}^{\;2} + 6\beta_i\beta_{iii} + 15\beta_{iii}^{\;2} + 24\beta_{ii}\beta_{iiii} + 96\beta_{iiii}^{\;2} + 30\beta_i\beta_{iiiii} + 210\beta_{iii}\beta_{iiiii} + 945\beta_{iiiii}^{\;2}\right) + \\
& \sum_{i=1}^{n}\sum_{\substack{j=1\\ i<j}}^{n}\left(\begin{array}{l}
\beta_{ij}^{\;2} + 3\beta_{iij}^{\;2} + 3\beta_{ijj}^{\;2} + 8\beta_{iijj}^{\;2} + 15\beta_{iiij}^{\;2} + 15\beta_{ijjj}^{\;2} + 45\beta_{iiijj}^{\;2} + 45\beta_{iijjj}^{\;2} + 105\beta_{iiiij}^{\;2} + 105\beta_{ijjjj}^{\;2} + 2\beta_i\beta_{ijj} + 2\beta_j\beta_{iij} + \\
4\beta_{ii}\beta_{iijj} + 4\beta_{jj}\beta_{iijj} + 6\beta_{ij}\beta_{iiij} + 6\beta_{ij}\beta_{ijjj} + 6\beta_i\beta_{ijjjj} + 6\beta_j\beta_{iiiij} + 6\beta_i\beta_{iiijj} + 6\beta_j\beta_{iijjj} + 6\beta_{iii}\beta_{ijj} + 6\beta_{jjj}\beta_{iij} + \\
24\beta_{iiii}\beta_{iijj} + 24\beta_{jjjj}\beta_{iijj} + 18\beta_{ijjj}\beta_{iiij} + 18\beta_{iii}\beta_{ijjjj} + 18\beta_{jjj}\beta_{iiiij} + 18\beta_{iij}\beta_{iijjj} + 18\beta_{ijj}\beta_{iiijj} + \\
30\beta_{iii}\beta_{iiijj} + 30\beta_{jjj}\beta_{iijjj} + 30\beta_{iij}\beta_{iiiij} + 30\beta_{ijj}\beta_{ijjjj} + 30\beta_{iij}\beta_{jjjjj} + 30\beta_{ijj}\beta_{iiiii} + \\
90\beta_{iiiii}\beta_{ijjjj} + 90\beta_{iiiij}\beta_{iijjj} + 90\beta_{iiiij}\beta_{jjjjj} + 90\beta_{iiijj}\beta_{ijjjj} + 210\beta_{iiiii}\beta_{iiijj} + 210\beta_{iijjj}\beta_{jjjjj}
\end{array}\right) + \\
& \sum_{i=1}^{n}\sum_{\substack{j=1\\ i<j}}^{n}\sum_{\substack{k=1\\ j<k}}^{n}\left(\begin{array}{l}
\beta_{ijk}^{\;2} + 3\beta_{iijk}^{\;2} + 3\beta_{ijjk}^{\;2} + 3\beta_{ijkk}^{\;2} + 9\beta_{iijjk}^{\;2} + 9\beta_{iijkk}^{\;2} + 9\beta_{ijjkk}^{\;2} + 15\beta_{iiijk}^{\;2} + 15\beta_{ijjjk}^{\;2} + 15\beta_{ijkkk}^{\;2} + \\
2\beta_i\beta_{ijjkk} + 2\beta_j\beta_{iijkk} + 2\beta_k\beta_{iijjk} + 2\beta_{ij}\beta_{ijkk} + 2\beta_{jk}\beta_{iijk} + 2\beta_{ik}\beta_{ijjk} + \\
2\beta_{iij}\beta_{jkk} + 2\beta_{iik}\beta_{jjk} + 2\beta_{ijj}\beta_{ikk} + 4\beta_{iijj}\beta_{jjkk} + 4\beta_{iijj}\beta_{iikk} + 4\beta_{iikk}\beta_{jjkk} + \\
6\beta_{iiij}\beta_{ijkk} + 6\beta_{iiik}\beta_{ijjk} + 6\beta_{ijjj}\beta_{ijkk} + 6\beta_{jjjk}\beta_{iijk} + 6\beta_{jkkk}\beta_{iijk} + 6\beta_{ikkk}\beta_{ijjk} + \\
6\beta_{iii}\beta_{ijjkk} + 6\beta_{jjj}\beta_{iijkk} + 6\beta_{kkk}\beta_{iijjk} + 6\beta_{ijk}\beta_{ijkkk} + 6\beta_{ijk}\beta_{ijjjk} + 6\beta_{ijk}\beta_{iiijk} + \\
6\beta_{iij}\beta_{iijkk} + 6\beta_{iij}\beta_{jjjkk} + 6\beta_{iij}\beta_{jkkkk} + 6\beta_{iik}\beta_{iijjk} + 6\beta_{iik}\beta_{jjjjk} + 6\beta_{iik}\beta_{jjkkk} + \\
6\beta_{ijj}\beta_{ijjkk} + 6\beta_{ijj}\beta_{iiikk} + 6\beta_{ijj}\beta_{ikkkk} + 6\beta_{jjk}\beta_{iijjk} + 6\beta_{jjk}\beta_{iiiik} + 6\beta_{jjk}\beta_{iikkk} + \\
6\beta_{ikk}\beta_{ijjkk} + 6\beta_{ikk}\beta_{iiiij} + 6\beta_{ikk}\beta_{ijjjj} + 6\beta_{jkk}\beta_{iijkk} + 6\beta_{jkk}\beta_{iiiij} + 6\beta_{jkk}\beta_{iijjj} + \\
18\beta_{iiiik}\beta_{jjjjk} + 18\beta_{iiiij}\beta_{jkkkk} + 18\beta_{ijjjj}\beta_{ikkkk} + 18\beta_{iiijk}\beta_{ijjjk} + 18\beta_{iiijk}\beta_{ijkkk} + 18\beta_{ijjjk}\beta_{ijkkk} + \\
18\beta_{iiiij}\beta_{jjjkk} + 18\beta_{iiiik}\beta_{jjkkk} + 18\beta_{ijjjj}\beta_{iiikk} + 18\beta_{jjjjk}\beta_{iikkk} + 18\beta_{ikkkk}\beta_{iiijj} + 18\beta_{jkkkk}\beta_{iijjj} + \\
18\beta_{iiijj}\beta_{ijjkk} + 18\beta_{iiikk}\beta_{ijjkk} + 18\beta_{iijjj}\beta_{iijkk} + 18\beta_{jjjkk}\beta_{iijkk} + 18\beta_{iikkk}\beta_{iijjk} + 18\beta_{jjkkk}\beta_{iijjk} + \\
30\beta_{iiiii}\beta_{ijjkk} + 30\beta_{jjjjj}\beta_{iijkk} + 30\beta_{kkkkk}\beta_{iijjk} + 30\beta_{iiijj}\beta_{iiikk} + 30\beta_{iijjj}\beta_{jjjkk} + 30\beta_{iikkk}\beta_{jjkkk} + \\
30\beta_{iiiij}\beta_{iijkk} + 30\beta_{iiiik}\beta_{iijjk} + 30\beta_{ijjjj}\beta_{ijjkk} + 30\beta_{jjjjk}\beta_{iijjk} + 30\beta_{ikkkk}\beta_{ijjkk} + 30\beta_{jkkkk}\beta_{iijkk}
\end{array}\right) + \\
& \sum_{i=1}^{n}\sum_{\substack{j=1\\ i<j}}^{n}\sum_{\substack{k=1\\ j<k}}^{n}\sum_{\substack{l=1\\ k<l}}^{n}\left(\begin{array}{l}
\beta_{ijkl}^{\;2} + 3\beta_{iijkl}^{\;2} + 3\beta_{ijjkl}^{\;2} + 3\beta_{ijkkl}^{\;2} + 3\beta_{ijkll}^{\;2} + \\
2\beta_{iikl}\beta_{jjkl} + 2\beta_{iijl}\beta_{jkkl} + 2\beta_{iijk}\beta_{jkll} + 2\beta_{ijjl}\beta_{ikkl} + 2\beta_{ijjk}\beta_{ikll} + 2\beta_{ijkk}\beta_{ijll} + \\
2\beta_{iij}\beta_{jkkll} + 2\beta_{iik}\beta_{jjkll} + 2\beta_{iil}\beta_{jjkkl} + 2\beta_{ijj}\beta_{ikkll} + 2\beta_{jjk}\beta_{iikll} + 2\beta_{jjl}\beta_{iikkl} + \\
2\beta_{ikk}\beta_{ijjll} + 2\beta_{jkk}\beta_{iijll} + 2\beta_{kkl}\beta_{iijjl} + 2\beta_{ill}\beta_{ijjkk} + 2\beta_{jll}\beta_{iijkk} + 2\beta_{kll}\beta_{iijjk} + \\
2\beta_{ijk}\beta_{ijkll} + 2\beta_{ijl}\beta_{ijkkl} + 2\beta_{ikl}\beta_{ijjkl} + 2\beta_{jkl}\beta_{iijkl} + \\
6\beta_{iiij}\beta_{jkkll} + 6\beta_{iiik}\beta_{jjkll} + 6\beta_{iiil}\beta_{jjkkl} + 6\beta_{ijjj}\beta_{ikkll} + 6\beta_{jjjk}\beta_{iikll} + 6\beta_{jjjl}\beta_{iikkl} + \\
6\beta_{ikkkk}\beta_{ijjll} + 6\beta_{jkkkk}\beta_{iijll} + 6\beta_{kkkkl}\beta_{iijjl} + 6\beta_{illll}\beta_{ijjkk} + 6\beta_{jllll}\beta_{iijkk} + 6\beta_{kllll}\beta_{iijjk} + \\
6\beta_{iiijj}\beta_{ikkll} + 6\beta_{iiikk}\beta_{ijjll} + 6\beta_{iiill}\beta_{ijjkk} + 6\beta_{iijjj}\beta_{jkkll} + 6\beta_{jjjkk}\beta_{iijll} + 6\beta_{jjjll}\beta_{iijkk} + \\
6\beta_{iikkk}\beta_{jjkll} + 6\beta_{jjkkk}\beta_{iikll} + 6\beta_{kkkll}\beta_{iijjk} + 6\beta_{iilll}\beta_{jjkkl} + 6\beta_{jjlll}\beta_{iikkl} + 6\beta_{kklll}\beta_{iijjl} + \\
6\beta_{iiijk}\beta_{ijkll} + 6\beta_{iiijl}\beta_{ijkkl} + 6\beta_{iiikl}\beta_{ijjkl} + 6\beta_{ijjjl}\beta_{ijkkl} + 6\beta_{ijjjk}\beta_{ijkll} + 6\beta_{jjjkl}\beta_{iijkl} + \\
6\beta_{ijkkk}\beta_{ijkll} + 6\beta_{ikkkl}\beta_{ijjkl} + 6\beta_{jkkkl}\beta_{iijkl} + 6\beta_{ijlll}\beta_{ijkkl} + 6\beta_{iklll}\beta_{ijjkl} + 6\beta_{jklll}\beta_{iijkl} + \\
6\beta_{ijjkk}\beta_{ijjll} + 6\beta_{ijjkk}\beta_{ikkll} + 6\beta_{ijjll}\beta_{ikkll} + 6\beta_{iijkk}\beta_{iijll} + 6\beta_{iijkk}\beta_{jkkll} + 6\beta_{iijll}\beta_{jkkll} + \\
6\beta_{iijjk}\beta_{iikll} + 6\beta_{iijjk}\beta_{jjkll} + 6\beta_{iikll}\beta_{jjkll} + 6\beta_{iijjl}\beta_{iikkl} + 6\beta_{iijjl}\beta_{jjkkl} + 6\beta_{iikkl}\beta_{jjkkl}
\end{array}\right) + \\
& \sum_{i=1}^{n}\sum_{\substack{j=1\\ i<j}}^{n}\sum_{\substack{k=1\\ j<k}}^{n}\sum_{\substack{l=1\\ k<l}}^{n}\sum_{\substack{m=1\\ m<k}}^{n}\left(\begin{array}{l}
\beta_{ijklm}^{\;2} + 2\beta_{ijjkk}\beta_{illmm} + 2\beta_{ijjll}\beta_{ikkmm} + 2\beta_{ijjmm}\beta_{ikkll} + \\
2\beta_{iijkk}\beta_{jllmm} + 2\beta_{iijll}\beta_{jkkmm} + 2\beta_{iijmm}\beta_{jkkll} + 2\beta_{iijjk}\beta_{kllmm} + 2\beta_{iikll}\beta_{jjkmm} + 2\beta_{iikmm}\beta_{jjkll} + \\
2\beta_{iijjl}\beta_{kklmm} + 2\beta_{iikkl}\beta_{jjlmm} + 2\beta_{iilmm}\beta_{jjkkl} + 2\beta_{iijjm}\beta_{kkllm} + 2\beta_{iikkm}\beta_{jjllm} + 2\beta_{iillm}\beta_{jjkkm}
\end{array}\right)
\end{aligned}
\tag{4.18}
$$

Totally 5,000 instances of polynomial response systems as defined in Equation 4.11 are simulated. For each instance of the response y, the exact transmitted variance is computed using Equation 4.18. Each of the methods to be compared provides an estimate of the transmitted variance whose error is computed by the comparison to the exact solution. The cumulative probability of the error for each method is then plotted in Figure 4.2. 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 a greater confidence that the given error tolerance will be satisfied than methods lower on the chart.

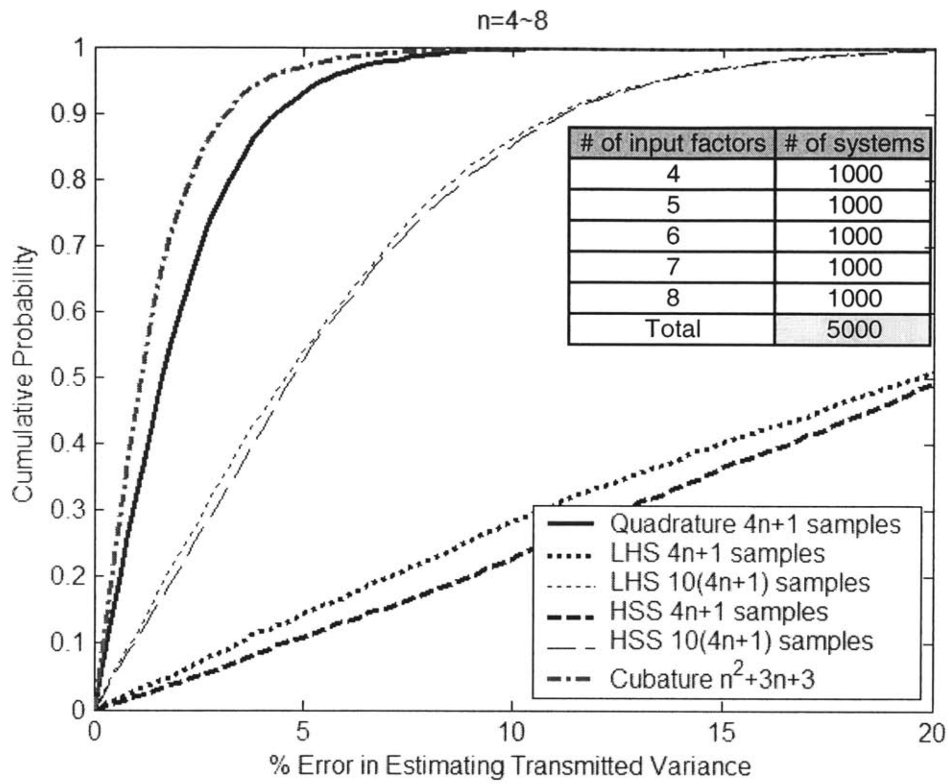


Figure 4.2 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to populations of 5th order polynomials of four to eight variables (n=4~8) whose polynomial coefficients decrease geometrically with order at rate $\sqrt{r}$ =0.2 for single factor effects and at a faster rate ($\sqrt{r_{INT}/r}=0.6$) for interaction effects. The Result is based on 5,000 systems generated from the Hierarchical Probability Model (Equations 4.11 to 4.16).

Figure 4.2 shows that the Hermite-Gaussian quadrature method estimates the transmitted variance within 5% error for more than 90% of all systems sampled. Hermite-Gaussian quadrature accomplishes this with only $4n+1$ samples. HSS and LHS are unable to provide comparably good results with comparable number of samples or even ten times number of samples. Lu and Darmofal's cubature method shows a slightly higher level of accuracy at the cost of a larger number of samples

(n^2+3n+3). This conclusion is draw from the average result (n=4~8). Appendix C shows five figures for n=4~8 separately. By observing the trend of LHS and HSS with ten times number of samples, we can infer that when n becomes large, LHS or HSS with ten times number of samples will likely have the same level of accuracy as the quadrature-based method. Due to computational difficulty, we only run simulation of fifth order polynomial up to n=8. It is a challenging task to hold 1000 matrix of β_{ijklm} when the numbers of input variables n is greater than 8. Current computers can easily run out of memory.

Appendix D shows that when the Hierarchical Probability Model (Equations 4.11 to 4.16) is reduced to a third order model, LHS and HSS with ten times number of samples have the same level accuracy as the quadrature-based method when n is greater than 13.

The accuracy of the Hermite-Gaussian quadrature method for un-separable, multi-variable, polynomial response systems seems to be reasonable for meeting practitioners' requirement in early stages of product development. A recent study of computer simulations has shown that merely porting an algorithm from one computer system to another frequently results in variations in the response greater than 5% (Hatton, 1997). Variations due to un-modeled physical effects and uncertainty of input parameters may be larger still. Therefore, it seems reasonable to require 5% accuracy in a sampling method given the presence of other, much larger, contributions to error.

The conclusions obtained from these two different probability models are somewhat similar. The underline effect hierarchy principle might account for this similarity. The first probability model presented in section 4.1 has been studied more extensively and parameters are specified, based on the study of 113 full factorial engineering experiments. Hence, it is recommend here to use the probability model in section 4.1 for lower-order, un-separable, multi-variable, response systems and only use the second probability model in section 4.2 for higher-order systems.

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

Chapter 5

Case Study

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

5.1 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 Hammersley Sequence Sampling (HSS) over Latin Hypercube Sampling (LHS) (Kalagnanam and Diwekar 1997). The function of the CSTR system is to produce a chemical species B at a target production rate (R_B) of 60 moles/minute. 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_{Ai} and C_{Bi}). The system is governed by five equations.

$$Q = F\rho C_p(T - T_i) + V(r_A H_{RA} + r_B H_{RB}) \tag{5.1}$$

$$C_A = \frac{C_{Ai}}{1 + k_A^0 e^{-E_A/RT}\tau} \tag{5.2}$$

$$C_B = \frac{C_{Bi} + k_A^0 e^{-E_A/RT}\tau C_A}{1 + k_B^0 e^{-E_B/RT}\tau} \tag{5.3}$$

$$-r_A = k_A^0 e^{-E_A/RT} C_A \tag{5.4}$$

$$-r_B = k_B^0 e^{-E_B/RT} C_B - k_A^0 e^{-E_A/RT} C_A \tag{5.5}$$

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

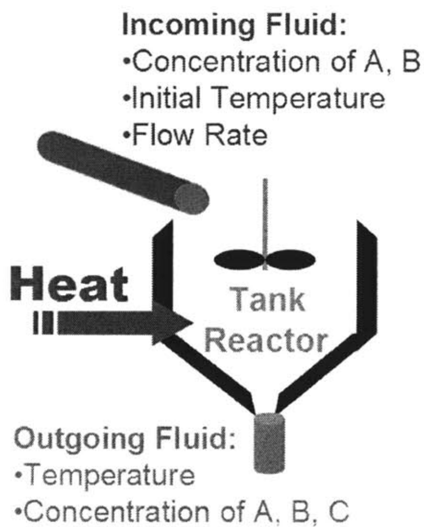


Figure 5.1 Continuous-Stirred Tank Reactor.

Table 5.1 provides a listing of physical constants, input and output variables. These values of physical constants and the input variables are taken directly from Kalagnanam and 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 is an initial design and the other is an optimized robust design, with greatly reduced variance in the response R_B.

To check that the model is correctly implemented, the results at both points are 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) and we compute a transmitted variance of 1625.7+1.5 (mol/min). There is also a small discrepancy in the transmitted variance of the robust design – the published value was 232 (mol/min) and we compute 232.3+0.4 (mol/min). The discrepancy between our results and the previously published results are small (less than 0.2%) and likely due to differences in implementation of the solver for the system of equations.

Monte Carlo simulations are run using 10^6 samples to estimate the true standard deviation of the response of the CSTR due to the 6 noise factors. Then, six different methods are used to estimate the transmitted variance of the response: 1) the quadrature-based method using $4n$+1 or 25 samples; 2) HSS using 25 samples (Systematically choose a total of 720 sets of different simulations); 3) LHS using 25 samples (randomly choose 1000 sets of different simulations); 4) Cubature using n^2+3n+3 or 57 samples; 5) HSS using 250 samples (Systematically choose a total of 720 sets of different simulations); and 6) LHS using 250 samples (randomly choose 1000 sets of different simulations).

TABLE 5.1 Parameters and their values in the CSTR 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

TABLE 5.2 Comparing the accuracy of sampling methods as applied to the continuous-stirred tank reactor.

Initial design				
Sampling method	**# of samples**	μ **(R_B)**	σ^2 **(R_B)**	**Error in estimate of** σ^2
Monte Carlo	10^6	60.434	1625.7	-----------
Quadrature	25	60.208	1455.3	10.5%*
HSS	25	[49.728 59.976]†	[1373.3 1704.5]†	6.9%**
LHS	25	[57.896 62.955]††	[1424.3 1986.1]††	8.9%**
Cubature	57	60.114	1502.6	7.8%*
HSS	250	[59.419 60.493]†	[1587.5 1656.3]†	1.0%**
LHS	250	[59.743 61.136]††	[1554.9 1719.9]††	2.5%**
Robust design				
Sampling method	**# of samples**	μ **(R_B)**	σ^2 **(R_B)**	**Error in estimate of** σ^2
Monte Carlo	10^6	50.894	232.3	----------
Quadrature	25	50.735	230.0	1.0%*
HSS	25	[48.558 52.580]†	[136.9 253.1]†	26.3%**
LHS	25	[49.088 52.551]††	[162.5 329.8]††	17.5%**
Cubature	57	50.621	238.8	2.8%*
HSS	250	[50.590 51.134]†	[218.9 241.2]†	2.8%**
LHS	250	[50.398 51.353]††	[212.7 254.6]††	4.5%**

† This range reports the range [5% 95%] of mean or variance of **(R_B)** based on 720=6! sets of different input samples for HSS with either 25 samples or 250 samples.

†† This range reports the range [5% 95%] of mean or variance of **(R_B)** based on 1000 sets of different input samples for LHS with either 25 samples or 250 samples.

* This value is the absolute value of the percentage error of σ^2. The formula used to obtain this value is $\frac{|\sigma^2 - \sigma^2_{Exact}|}{\sigma^2_{Exact}}$.

**This value is the *averaged* absolute value of the percentage error of σ^2 based on the 1000 simulations of LHS with 25 or 250 samples, or based on the 720 simulations of HSS with 25 or 250 samples. The formula used to obtain this value is $\overline{\left(\frac{|\sigma^2 - \sigma^2_{Exact}|}{\sigma^2_{Exact}}\right)}$.

Table 5.2 presents the results. The error of the quadrature technique as applied to the CSTR is about 10% for the initial design and improves substantially when the design is made more robust. HSS and LHS with 25 samples outperform quadrature at the initial design, but then perform very poorly at the robust design. Although cubature with about twice number of samples outperforms quadrtaure for the initial design, it underperforms the quadrature technique for the robust design.

5.2 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 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.

$$\boldsymbol{F}_{tot} = -m(\mu / R^2)\boldsymbol{e}_R + \frac{1}{2}\rho v_r^2 A_{ref} c_d \boldsymbol{e}_d \tag{5.6}$$

$$\rho \approx \rho_0 \cdot \exp\left[-(h-h_o)/h_s\right] \tag{5.7}$$

$$\mu = gR_0^2 \tag{5.8}$$

Table 5.3 provides a listing of physical constants and nine dispersed vehicle and environmental parameters. 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 is performed. Mistree et al. (1993) found the landing position of -106.65 degrees longitude and 33.71 degrees latitude. We obtain -106.65 degrees longitude and 33.69 degrees latitude.

Monte Carlo simulations are run using 10^4 samples to estimate the true standard deviation of both landing longitude and latitude due to the 9 noise factors. Then, six different methods are used to estimate the transmitted variance of the response: 1) the quadrature-based method using $4n$+1 or 37 samples; 2) HSS using 37 samples (randomly choose 1000 sets of different simulations); 3) LHS using 37 samples (randomly choose 1000 sets of different simulations); 4) Cubature using n^2+3n+3 or 111 samples; 5) HSS using 370 samples (randomly choose 1000 sets of different simulations); and 6) LHS using 370 samples (randomly choose 1000 sets of different simulations).

Table 5.4 presents the results for the longitude landing position and table 5.5 presents the results for the latitude landing position. Both the quadrature-based technique and cubature are excellent in estimating the transmitted variances of longitude landing positions of the initial design and robust design. For estimating the latitude landing position of the initial design, the error of quadrature-based technique and cubature are both small (1.7% for quadrature and 1.5% for cubature). Although the quadrature deteriorates slightly as the design is made more robust, it still outperforms the LHS with ten times number of samples.

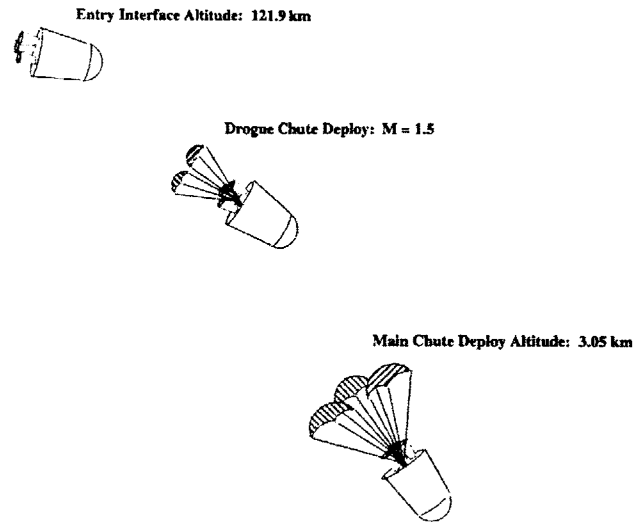


Figure 5.2 LifeSat Satellite (from Mistree, et al. 1993).

TABLE 5.3 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	121920 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

TABLE 5.4 Comparing the accuracy of sampling methods as applied to the LifeSat Satellite (Longitude).

Initial design				
Sampling method	**# of samples**	μ	σ^2 $(\times 10^{-4})$	**Error in estimate of σ^2**
Monte Carlo	10^4	-106.6508	37	---------
Quadrature	37	-106.6504	37	0.0%*
HSS	37	[-106.665, -106.651] †	[30, 38] †	10.6%**
LHS	37	[-106.651, -106.649] ††	[34, 43] ††	6.1%**
Cubature	111	-106.65	37	0.0%*
HSS	370	[-106.652, -106.651] †	[36, 37] †	0.9%**
LHS	370	[-106.650, -106.650] ††	[36, 37] ††	1.0%**
Robust design				
Sampling method	**# of samples**	μ	σ^2 $(\times 10^{-4})$	**Error in estimate of σ^2**
Monte Carlo	10^4	-106.6501	1.4884	--------
Quadrature	37	-106.65	1.4884	0.0%*
HSS	37	[-106.653, -106.650] †	[1.210 1.664] †	14.3%**
LHS	37	[-106.650, -106.650] ††	[1.145 1.960] ††	13.5%**
Cubature	111	-106.65	1.4884	0.0%*
HSS	370	[-106.651, -106.650] †	[1.440 1.488] †	5.5%**
LHS	370	[-106.650, -106.650] ††	[1.440 1.538] ††	3.7%**

† This range reports the range [5% 95%] of mean or variance based on 1000 sets of different input samples for HSS with either 25 samples or 250 samples (total possible different input samples are 362,880 $=n!=9!$).

†† This range reports the range [5% 95%] of mean or variance based on 1000 sets of different input samples for LHS with either 25 samples or 250 samples.

* This value is the absolute value of the percentage error of σ^2. The formula used to obtain this value is $\frac{|\sigma^2 - \sigma^2_{Exact}|}{\sigma^2_{Exact}}$.

**This value is the *averaged* absolute value of the percentage error of σ^2 based on the 1000 simulations of LHS with 25 or 250 samples, or based on the 1000 simulations of HSS with 25 or 250 samples. The formula used to obtain this value is $\overline{\left(\frac{|\sigma^2 - \sigma^2_{Exact}|}{\sigma^2_{Exact}}\right)}$.

TABLE 5.5 Comparing the accuracy of sampling methods as applied to the LifeSat Satellite (Latitude).

Initial design				
Sampling method	**# of samples**	μ	σ^2	**Error in estimate of σ^2**
Monte Carlo	10^4	33.6093	0.4492	---------
Quadrature	37	33.6104	0.4414	1.7%*
HSS	37	[33.6037 33.7661]†	[0.3534 0.4532]†	15.2%**
LHS	37	[33.5944 33.6241]††	[0.3930 0.5433]††	8.0%**
Cubature	111	33.6101	0.4423	1.5%*
HSS	370	[33.6102 33.6292]†	[0.4245 0.4439]†	8.2%**
LHS	370	[33.6072 33.6112]††	[0.4306 0.4549]††	6.0%**
Robust design				
Sampling method	**# of samples**	μ	σ^2	**Error in estimate of σ^2**
Monte Carlo	10^4	33.6983	0.0487	--------
Quadrature	37	33.6986	0.0505	3.7%*
HSS	37	[33.6676 33.7303]†	[0.0334 0.0541]†	10.5%**
LHS	37	[33.6923 33.7041]††	[0.0343 0.0692]††	16.6%**
Cubature	111	33.6982	0.0495	1.6%*
HSS	370	[33.6942 33.7014]†	[0.0468 0.0511]†	2.4%**
LHS	370	[33.6979 33.6986]††	[0.0481 0.0531]††	5.2%**

†, ††, *, and ** : The definitions are the same as those in Table 5.4.

5.3 I Beam

The engineering system in this case is an I beam (Figure 1.1) which was used to demonstrate the advantages of dimension reduction integration in uncertainty analysis (Huang and Du 2005). The system is governed by the following three equations

$$Y = g(X) = \sigma_{\max} - S \tag{5.9}$$

$$\sigma_{\max} = \frac{Pa(L-a)d}{2L \cdot I} \tag{5.10}$$

$$I = \frac{b_f d^3 - (b_f - t_w)(d - 2t_f)^3}{12} \tag{5.11}$$

Table 5.6 provides a listing of eight random variables which are taken directly from the published case study (Huang and Du 2005). We consider two different designs: one is an initial design from the published case, and the other is an optimized robust design proposed here, with greatly reduced variance in the output performance.

To check that the model is correctly implemented, the results at both points are reproduced by Monte Carlo simulations with 10^6 trials each. Huang and 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 computes 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 are 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 are used to estimate the transmitted variance of the response: 1) the quadrature-based method using $4n+1$ or 33 samples; 2) HSS using 33 samples (randomly choose 1000 sets of different simulations); 3) LHS using 33 samples (randomly choose 1000 sets of different simulations); 4) Cubature using n^2+3n+3 or 91 samples; 5) HSS using 330 samples (randomly choose 1000 sets of different simulations); and 6) LHS using 330 samples (randomly choose 1000 sets of different simulations).

Table 5.7 presents the results of the case study. The accuracy of the quadrature-based technique as applied to the I beam is excellent beginning at less than 2% error and improves as the design is made more robust. This level of accuracy is superior to LHS and HSS using a comparable number of samples. If HSS or LHS is afforded ten times the number of samples as quadrature, it could also provide excellent accuracy, but the quadrature-based method is superior with comparable number of samples.

TABLE 5.6 Parameters and their values in the I beam case study.

Initial design		
Parameter	**Mean**	**Standard Deviation**
P	6070	200
L	120	6
a	72	6
S	170000	4760
d	2.3	1/24
b_f	2.3	1/24
t_w	0.16	1/48
t_f	0.26	1/48
Robust design		
P	10125	200
L	240	6
a	109	6
S	85000	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 5.7 Comparing the accuracy of sampling methods as applied to the I beam.

Initial design				
Sampling method	**# of samples**	μ	σ^2 ($\times 10^8$)	**Error in estimate of σ^2**
Monte Carlo	10^6	-19825	3.2048	---------
Quadrature	33	-19805	3.1407	2.0%*
HSS	33	[-20725, -16374] †	[1.8550, 3.7561] †	14.1%**
LHS	33	[-20684, -19024] ††	[2.1346, 4.6536] ††	19.2%**
Cubature	73	-19819	3.2095	0.1%*
HSS	330	[-19925, -19169] †	[2.8459, 3.3095] †	2.9%**
LHS	330	[-20017, -19603] ††	[2.8769, 3.5615] ††	5.5%**
Robust design				
Sampling method	**# of samples**	μ	σ^2 ($\times 10^8$)	**Error in estimate of σ^2**
Monte Carlo	10^6	-19818	3.0644	---------
Quadrature	33	-19825	3.0663	0.1%*
HSS	33	[-19868, -18554] †	[2.3013, 3.3224] †	10.9%**
LHS	33	[-19970, -19658] ††	[2.3069, 4.1298] ††	14.8%**
Cubature	73	-19825	3.0658	0.1%*
HSS	330	[-19831, -19603] †	[2.8903, 3.1086] †	2.2%**
LHS	330	[-19842, -19804] ††	[2.8088, 3.3405] ††	4.2%**

†, ††, *, and ** : The definitions are the same as those in Table 5.4.

5.4 Ten-Bar Truss

The engineering system in this case is a linear-elastic ten-bar truss structure which was used to demonstrate the accuracy and efficiency of the univariate approximation method in higher-order reliability analysis (Rahman and Wei 2005). Two concentrated forces are applied at nodes 2 and 3 of the structure as indicated in Figure 5.3. The maximum displacement occurs at node 3b 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 non-linear behavior of the structure.

Table 5.8 provides a listing of physical constants and ten random variables which are taken from the published case (Rahman and Wei 2005). We consider two different designs: one is an initial design given in the published case and the other is an optimized robust design proposed here, which greatly reduces variance in the output performance.

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

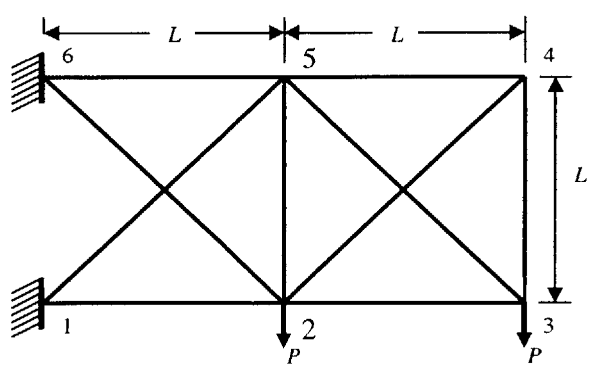


Figure 5.3 A Ten-Bar truss structure (from Rahman and Wei 2005).

TABLE 5.8 Parameters and their values in the Ten-Bar Truss case study.

Parameter	Value	Units
Young's modulus E	10^7	psi
Load P	10^5	lb
Length L	360	in
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

Monte Carlo simulations are run using 10^6 samples to estimate the true standard deviation of the output performance due to the ten noise factors. Then, six different methods are used to estimate the transmitted variance of the response: 1) the quadrature-based method using $4n+1$ or 41 samples; 2) HSS using 41 samples (randomly choose 1000 sets of different simulations); 3) LHS using 41 samples (randomly choose 1000 sets of different simulations); 4) Cubature using n^2+3n+3 or 133 samples; 5) HSS using 410 samples (randomly choose 1000 sets of different simulations); and 6) LHS using 410 samples (randomly choose 1000 sets of different simulations).

Table 5.9 presents the results. The error of the quadrature-based technique as applied to the ten-bar truss is less than 6% for both the initial design and the robust design. This level of accuracy is superior to LHS and HSS using a comparable number of samples. If HSS and LHS are afforded ten times the number of samples as quadrature, they could also provide same level of accuracy, but the quadrature–based technique is superior with comparable number of samples. Note that in this case study, the standard deviation of the noise factor is 20% of the mean whereas in most other case studies, the standard deviation of the noise factor is less than 10% of the mean. If the standard deviation were restricted to 0.25 inches for each bar, the error of quadrature as applied to the ten-bar truss would be smaller than 1%. However, we do not want to change the character of the published case study. Instead, we subject our results to the more difficult test presented by this case study.

TABLE 5.9 Comparing the accuracy of sampling methods as applied to the ten-bar truss.

Initial design				
Sampling method	**# of samples**	μ	σ^2	**Error in estimate of σ^2**
Monte Carlo	10^6	16.3225	2.6680	---------
Quadrature	41	16.3145	2.5322	5.1%*
HSS	41	[16.614, 16.962] †	[1.689, 3.479] †	17.2%**
LHS	41	[16.256, 16.416] ††	[1.903, 3.787] ††	18.2%**
Cubature	133	16.3138	2.4530	4.1%*
HSS	410	[16.380, 16.446] †	[2.442, 2.868] †	4.2%**
LHS	410	[16.307, 16.339] ††	[2.345, 2.965] ††	5.8%**
Robust design				
Sampling method	**# of samples**	μ	σ^2	**Error in estimate of σ^2**
Monte Carlo	10^6	16.3330	2.2807	---------
Quadrature	41	16.3225	2.1521	5.6%*
HSS	41	[16.656, 16.954] †	[1.406, 2.903] †	17.6%**
LHS	41	[16.266, 16.414] ††	[1.507, 3.345] ††	19.6%**
Cubature	133	16.3256	2.1857	4.2%*
HSS	410	[16.397, 16.448] †	[2.080, 2.405] †	4.1%**
LHS	410	[16.316, 16.348] ††	[2.030, 2.536] ††	5.3%**

†, ††, *, and ** : The definitions are the same as those in Table 5.4.

5.5 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 5.4. The op-amp is to be manufactured on a single board using fifteen circuit elements whose parameters are to be chosen so that the offset voltage of the circuit is consistent despite manufacturing variations. There are twenty-one noise factors which affect the offset voltage (twenty characterizing the circuit elements and one for the operating temperature) as shown in Table 5.10. Following the example of Phadke, we modeled some of the noise factors as correlated and some as independent. 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 5.10 (Phadke 1989).

We developed a simulation of the op amp circuit based on an Ebers-Moll model of the transistors. Monte Carlo simulations are run using 3×10^4 samples to estimate the true transmitted variance of the response of the op amp due to the 21 noise factors. Then, six different methods are used to estimate the transmitted variance of the offset voltage: 1) the quadrature technique using $2n+1$ or 43 samples; 2) HSS using 43 samples (randomly choose 1000 sets of different simulations); 3) LHS using 43 samples (randomly choose 1000 sets of different simulations); 4) Cubature using $n^2 + 3n + 3$ or 507 samples; 5) HSS using 430 samples (randomly choose 1000 sets of different simulations); and 6) LHS using 430 samples (randomly choose 1000 sets of different simulations).

Table 5.11 presents the results of the case study. This case study has the largest number of noise factors comparing to other case studies in this chapter. The accuracy of the quadrature-based technique as applied to the op amp is excellent beginning at about 1% error and deteriorates slightly as the design is made more robust. This level of accuracy is superior to any other alternative method using a comparable number of samples or ten times number of samples in both initial design and robust design.

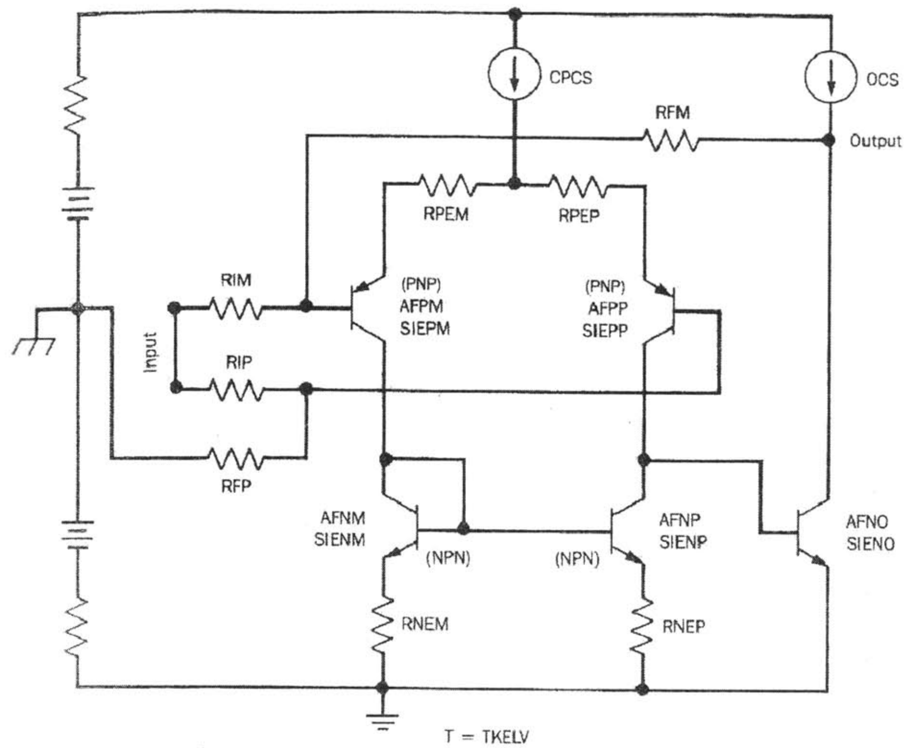


Figure 5.4 Differential Op Amp Circuit Diagram (from Phadke 1989).

TABLE 5.10 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

TABLE 5.11 Comparing the accuracy of sampling methods as applied to the operational amplifier.

Initial design				
Sampling method	**# of samples**	μ	σ^2	**Error in estimate of σ^2**
Monte Carlo	$3X10^4$	-2.754	916.33	---------
Quadrature	43	-2.755	906.37	1.1%*
HSS	43	[-16.723 -1.00] †	[349.8 1079.5] †	25.2%**
LHS	43	[-3.355 -1.672] ††	[736.4 1274.8] ††	16.0%**
Cubature	507	-2.763	902.88	1.5%*
HSS	430	[-5.113 -2.407] †	[896.1 1111.0] †	7.2%**
LHS	430	[-2.743 -2.232] ††	[885.7 1086.7] ††	9.0%**
Robust design				
Sampling method	**# of samples**	μ	σ^2	**Error in estimate of σ^2**
Monte Carlo	$3X10^4$	-1.635	371.95	---------
Quadrature	43	-1.612	359.03	3.5%*
HSS	43	[-9.470 0.704] †	[94.6 383.28] †	33.4%**
LHS	43	[-2.055 -0.930] ††	[274.2 490.58] ††	16.8%**
Cubature	507	-1.610	348.64	6.3%*
HSS	430	[-2.878 -1.193] †	[338.6 423.59] †	7.0%**
LHS	430	[-1.691 -1.325] ††	[334.9 426.54] ††	6.3%**

†, ††, *, and ** : The definitions are the same as those in Table 5.4.

5.6 All the Case Studies as a Set

The set of case studies presented in the previous five subsections can be studied as a set. There were five engineering systems with 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 cumulative density function (cdf) of its accuracy. These empirical cdfs are presented in Figure 5.5 with the hierarchical probability model (Equations 4.11 to 4.16) based cdf for the $4n$+1 quadrature technique as previously presented in Figure 4.2.

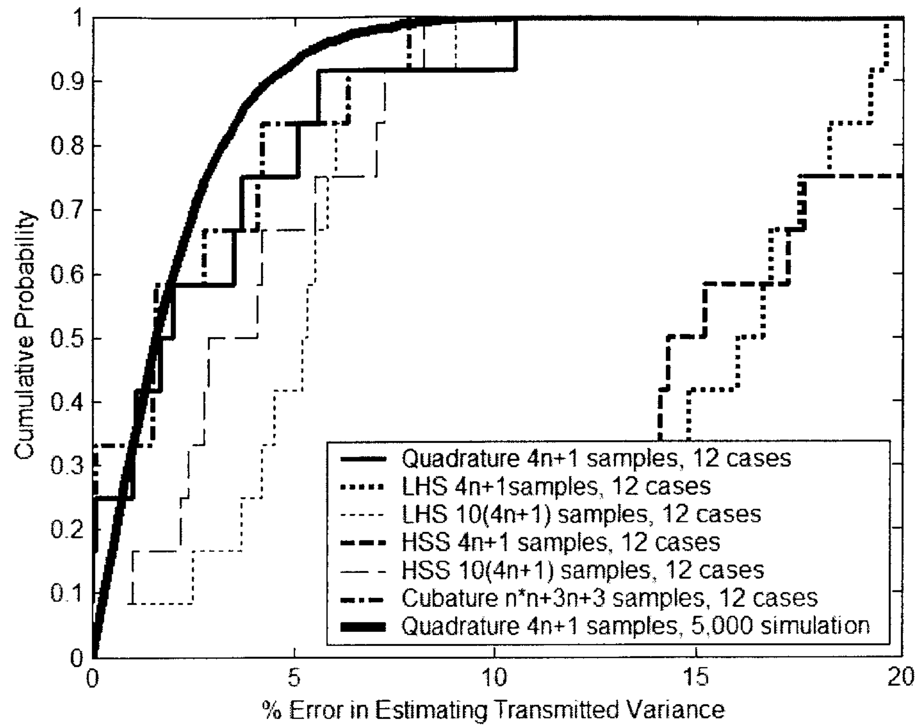


Figure 5.5 Empirical cumulative density functions based on the set of case studies. The model-based cumulative density functions of the $4n+1$ quadrature technique is provided for comparison.

A principal observation is that, for the $4n+1$ quadrature technique, the empirical cdf largely matches the model-based cdf. In the range of 2-10% accuracy, the empirical cdfs indicate a somewhat lower probability than the model-based cdfs. 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.

Overall, the case studies as a set are consistent with the principal claims from the hierarchical probability model (Equations 4.11 to 4.16). The quadrature technique enables a ten-fold reduction in the number of computational simulations needed for robust design while providing reasonable accuracy.

Figure 5.6 shows a complete comparison of the empirical cdfs and the hierarchical probability model (Equations 4.11 to 4.16) based cdfs.

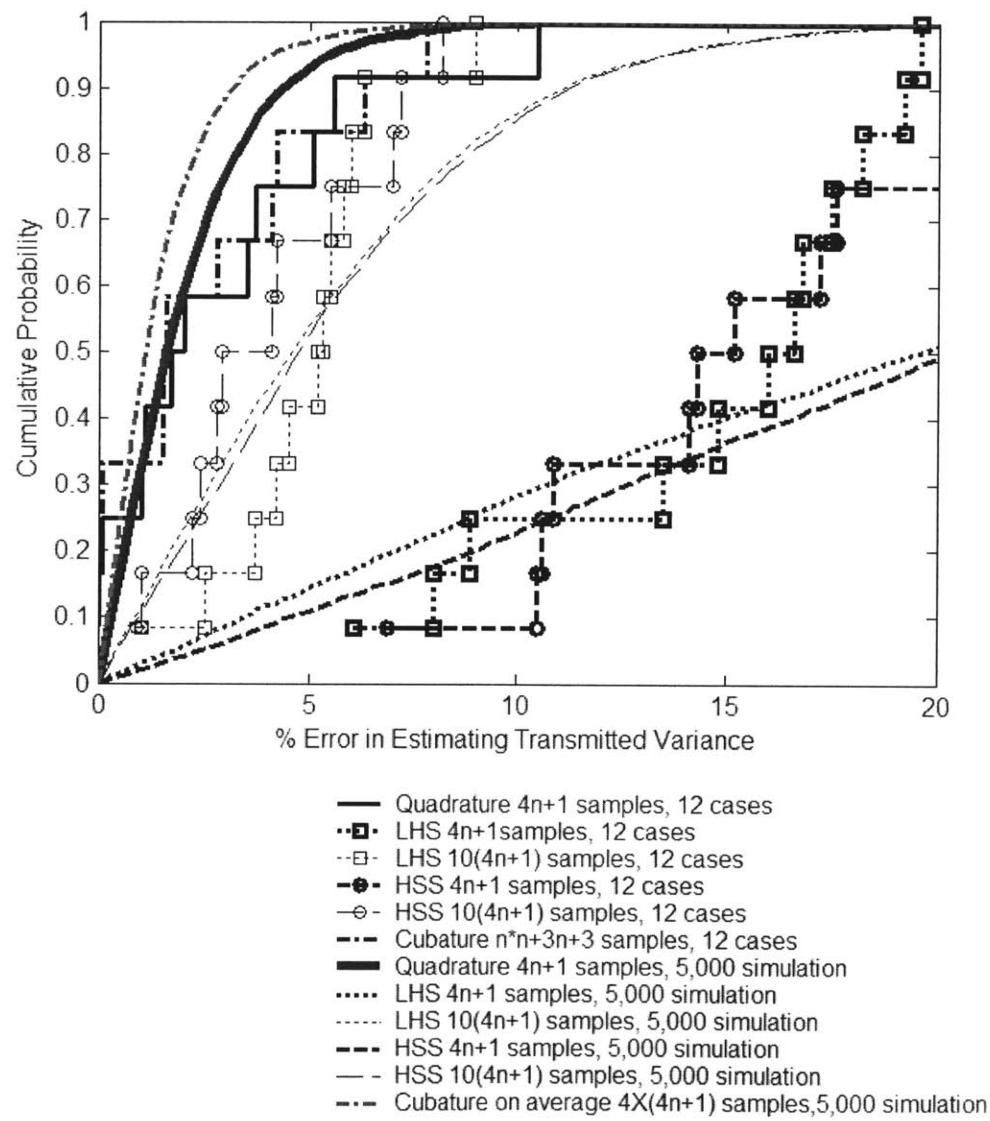


Figure 5.6 : Empirical cumulative density functions based on the set of case studies. The model-based cumulative density functions are provided for comparison.

The comparison of empirical cdfs and cdfs based on the hierarchical probability model (Equations 4.1 to 4.8) is NOT plotted. The reason is that the parameters in the hierarchical probability model (Equations 4.1 to 4.8) should be further calibrated to address the issue of the mismatch between the empirical cdfs and the model-based cdfs for Lu and Darmofal cubature method.

Chapter 6

Conclusions

The main results and contributions of this thesis are summarized as follows:

This thesis provides an alternative tool for practitioners to efficiently estimate the transmitted variance. This tool is based on the 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 thesis 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 1) the method gives exact transmitted variance if the response is up to a fourth-order separable polynomial response and 2) the error of the transmitted variance estimated by the method is smaller than zero if the response is a fifth-order separable polynomial response.

In addition, this thesis provides an evaluation of **un-separable** polynomial response systems by comparing the accuracy of the transmitted variance using the quadrature-based method and alternative sampling methods. The advantages of the quadrature-based method have been 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 cases. The proposed method provides much better accuracy than Latin Hypercube Sampling or Hammersley Sequence Sampling, assuming these techniques are also restricted to using $4n+1$ samples. Only if Hammersley Sequence Sampling is afforded at least ten times the number of samples, can it provide approximately the same degree of accuracy as the quadrature technique. 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 quadrature-based method adds value to the practitioner's toolbox. When practitioners face engineering problems with *more* separability, a slow rate of decay of nonlinear effects, and *larger* numbers of input variables, the quadrature-based method can give the transmitted variance efficiently and accurately. When practical engineering problems have *less* separability, a *fast* rate of decay of nonlinear effects, and *smaller* numbers of input variables, the cubature method is the preferable choice. When practical engineering problems have *more* separability, a fast rate of decay of nonlinear effects, and *larger* numbers of input variables, the FOSM or SOSM is the preferable choice.

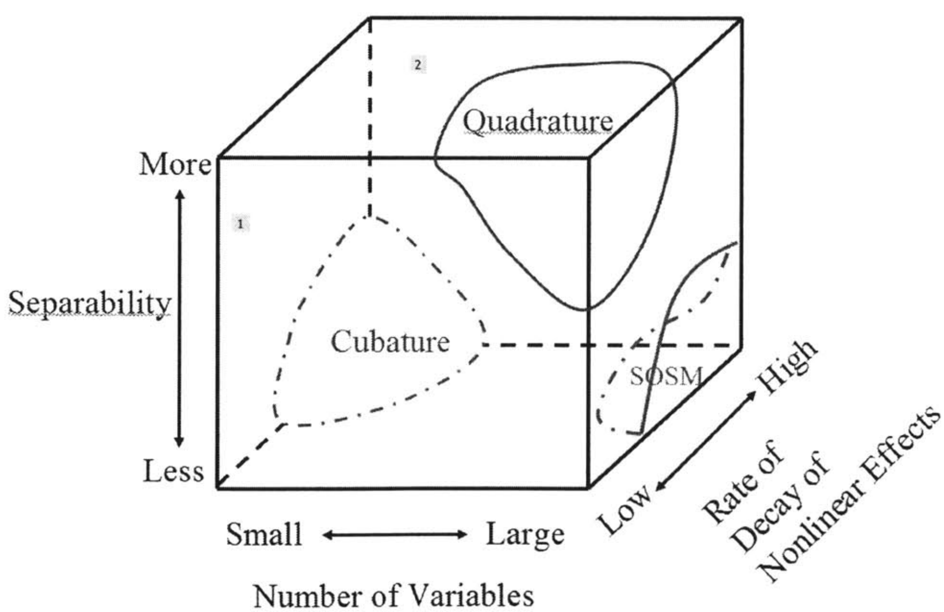


Figure 6.1 The comparison of the quadrature-based method, cubature, and SOSM.

References

Booker, A. J., Dennis, J. E., Jr., F., P. D., Serafini, D. B., Torczon, V., and Trosset, M. W., 1999, "A Rigorous Framework for Optimization of Expensive Functions by Surrogates." Structural Optimization, 17(1), 1-13

Chipman, H. M., M. Hamada, and C. F. J. Wu, 1997, "Bayesian variable-selection approach for analyzing designed experiments with complex aliasing," *Technometrics* **39**(4) 372-381.

Christoffel, E. B., 1877, "Sur une classe particuliere de functions entieres et de fractions continues," *Annali di Matematica Pura ed Applicata*, series 2, vol. 8, pp. 1-10.

Cools, R., 1999, "Monomial Cubature Rules Since "Stroud": A Compilation – Part 2," *Journal of Computational and Applied Mathematics* **112**: 21-27.

Cools, R., P. Rabinowitz, 1993, "Monomial Cubature Rules Since "Stroud": A Compilation," *Journal of Computational and Applied Mathematics* **48**(3): 309-326.

Diwekar U. M., 2003, "A novel sampling approach to combinatorial optimization under uncertainty" *Computational Optimization and Applications* 24 (2-3): 335-371.

Du, X., and Chen, W., 2002, "Sequential Optimization and Reliability Assessment Method for Efficient Probabilistic Design," ASME Design Automation Conference.

Du, X., Sudjianto, A., and Chen, W., 2004, "An Integrated Framework for Optimization Under Uncertainty Using Inverse Reliability Strategy," ASME Journal of Mechanical Design, 126, 1–9.

Frey D., Reber G. S., and Lin, Y., 2005, "A Quadrature-based Technique for Robust Design with Computer Simulations," ASME Design Engineering Technical Conferences, Sept. 24-28, Long Beach, CA.

Fieller, E. C., 1932, The distribution of the index in a normal bivariate population. *Biometrika* **24**, pp. 428-40.

Gauss, 1814, "Methodus nova integralium valores per approximationem inveniendi," *Comment. Soc. Regiae Sci. Gottiningensis Recentiores*, vol. 3, pp. 202-206.

Gautchi, W., 1983, "How and How Not to Check Gaussian Quadrature Formulae," BIT 23 209-216.

Gautchi, W., 1968, "Construction of Gauss-Christoffel Quadrature Formulas," Mathematics of Computation 22 102 251-270.

Giunta, A.A., Wojtkiewicz, S.F., Jr., and Eldred, M.S., 2003, "Overview of Modern Design of Experiments Methods for Computational Simulations," *AIAA 2003-0649, 41st AIAA Aerospace Sciences Meeting and Exhibit*, Reno, NV.

Hatton, L., 1997, "The T-experiments in Quality of Numerical Software, Assessment and Enhancement," *IEEE Computational Science & Engineering*, **4**(2), 27-38.

Hazelrigg, G., 2003, "Thoughts on Model Validation for Engineering Design," *Proceedings of the ASME Design Theory and Methodology Conference*, Chicago, IL, DETC2003/DTM-48632.

Huang, B. and Du, X. 2005, "Uncertainty analysis by dimension reduction integration and saddlepoint approximations," ASME Design Engineering Technical Conferences, Sept. 24-28, Long Beach, CA.

Hoffman, R.M., Sudjianto, A., Du, X., and Stout, J., 2003, "Robust Piston Design and Optimization Using Piston Secondary Motion Analysis," SAE 2003 World Congress

Joseph, V. R., 2006, "A Bayesian approach to the design and analysis of fractionated experiments," Technometrics, v 48, n 2, p 219-229.

Kalagnanam, J. R. and U. M. Diwekar, 1997, "An Efficient Sampling Technique for Off-Line Quality Control", Technometrics 39(3)308-319.

Koch, P. N., Yang, R.-J., and Gu, L., 2004, "Design for Six Sigma Through Robust Optimization" Structural and Multidisciplinary Optimization

Li, R. and Sudjianto, A., 2005, "Analysis of Computer Experiments Using Penalized Like-lihood in Gaussian Kriging Models", Technometrics, v47, p111-p120.

Li, X. and Frey D., 2005, "Study of Effect Structures in Engineering Systems," ASME Design Engineering Technical Conferences, Sept. 24-28, Long Beach, CA.

Lu, J. L., and Darmofal, D., 2005, "Numerical Integration in Higher Dimensions with Gaussian Weight Function for Application to Probabilistic Design," SIAM Journal of Scientific Computing, 26 (2) 613-624.

James, L.A. and Oldenburg, M.C., 1997. Linear and Monte Carlo uncertainty analysis for subsurface contaminant transport simulation. Water Resour. Res. **33** 11, pp. 2495–2508.

Jin R, Chen W, Simpson T.W., 2000, "Comparative studies of metamodeling techniques under multiple modeling criteria," Technical Report 2000—4801, AIAA

Magnus, J., 1986, "The Exact Moments of a Ratio of Quadratic Forms of Normal Variables", Annales d'Economie et de Statistique, 4, pp. 95-109.

Manteufel, R. D., 2000, "Evaluating the Convergence of Latin Hypercube Sampling", AIAA-2000-1636, 41st AIAA Structures, Structural Dynamics, and Materials Conference, Atlanta, GA, 3-8 April.

McKay, M.D., R. J. Beckman, and W. J. Conover, 1979, "Comparison of three methods for selecting values of input variables in the analysis of output from a computer code," Technometrics 21(2)239-245.

Malkawi A. I. H., Hassan W.F., Abdulla F.A, 2000, "Uncertainty and reliability analysis applied to slope stability" Structural Safety 22 161-187

Mistree, F., Lautenschläger,U., Erikstad, S. O. ,and Allen, J. K.,1993, "Simulation reduction using the Taguchi method," Contractor Report 4542, NASA.

Phadke, Madhav S., 1989, Quality Engineering Using Robust Design, Prentice Hall, Englewood Cliffs, NJ.

Rahman, S. and Wei D. 2005, "A univariate approximation at most probable point for higher-order reliability analysis" Submitted to International Journal of Solids and Structures.

Reber G. S. 2004 Gaussian Quadrature for Computer Aided Robust Design. Master's Thesis, Massachusetts Institute of Technology.

Santner, T. J., B. J. Williams, and W. Notz, 2003, The Design and Analysis of Computer Experiments, Springer-Verlag, New York.

Seo, H. S. and Kwak, B. M., 2002, "Efficient statistical tolerance analysis for general distributions using three-point information," int. j. prod. res., 2002, vol. 40, no. 4, 931±944

Simpson, T.W.; Peplinski, J.; Koch, P. N.; and Allen, J.K., 2001, "Meta-models for Computer-based Engineering Design: Survey and Recommendations," Engineering with Computers 17(2)129-150.

Solari G. and Piccardo G., 2001, "Probabilistic 3D turbulence modeling for gust buffeting of structures", Prob. Eng. Mech. **16** , pp. 73–86

Stroud, A. H., 1971, Approximate Calculation of Multiple Integrals, Prentice Hall Series in Automatic Computation, Englewood Cliffs, NJ.

Stroud, A. H., and D. Seacrest, 1966, Gaussian Quadrature Formulas, Prentice Hall, Englewood Cliffs, NJ.

Taguchi, G., 1987, System of Experimental Design: Engineering Methods to Optimize Quality and Minimize Costs, American Supplier Institute, Dearborn, MI.

Wang, L., Beeson, D., and Wiggs, G., 2004, "Efficient and Accurate Point Estimate Method for Moments and Probability Distribution," 10th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, August 30 - September 1, 2004, Albany, New York.

Wu, C.F.J., and Hamada, M., 2000, Experiments: Planning, Analysis, and Parameter Design Optimization, Wiley &Sons, Inc., NY.

Ye, K. Q., Li, W., and Sudjianto, A., 2000, "Algorithmic Construction of Optimal Symmetric Latin Hypercube Designs," Journal of Statistical Planning and Inference, 90, 145–159.

Appendix A: <u>A detail examination of cumulative probability versus relative error in estimating transmitted variance for the Hierarchical Probability Model (Equations 4.11 to 4.16).</u>

Figure 4.2 shows the average result (n=4~8) of cumulative probability versus relative error in estimating transmitted variance for the hierarchical probability model - Equations 4.11 to 4.16. From Figure 4.2, we can see that the quadrature-base method is better than LHS and HSS with 10 times number of samples. This Appendix A shows figures for n=4~8 separately. Based on a detail examination of each plot for n=4~8, we find some trends. We can infer that when n becomes large, LHS or HSS with ten times number of samples will likely have the same level accuracy as the quadrature-based method. This is reasonable. Because when n is large (n>8), LHS or HSS with ten times number of samples requires over 400 samples. Both LHS and HSS are likely becoming more accurate when the samples points increase, because they are sampling methods based on the large sample properties.

A variety of alternative procedures applied to populations of 5th order polynomials whose polynomial coefficients decrease geometrically with order at rate $\sqrt{r}$ =0.2 for single factor effects and at a faster rate ($\sqrt{r_{INT}/r} = 0.6$) for interaction effects. Each Figure is based on a population of 1,000 systems generated from the Hierarchical Probability Model (Equations 4.11 to 4.16).

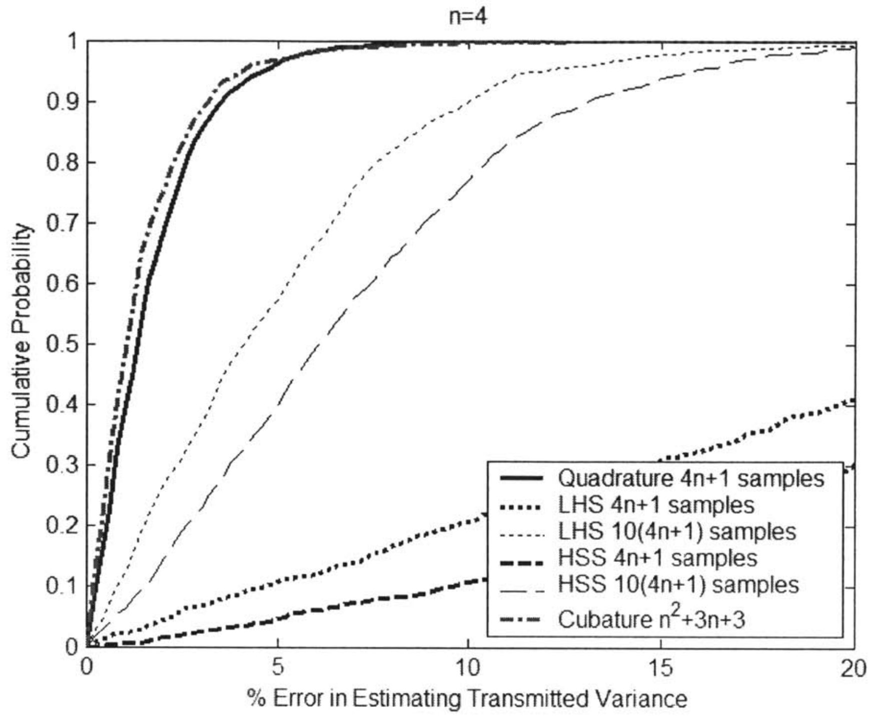


Figure A.1 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 5^{th} order polynomials of four inputs (n=4)

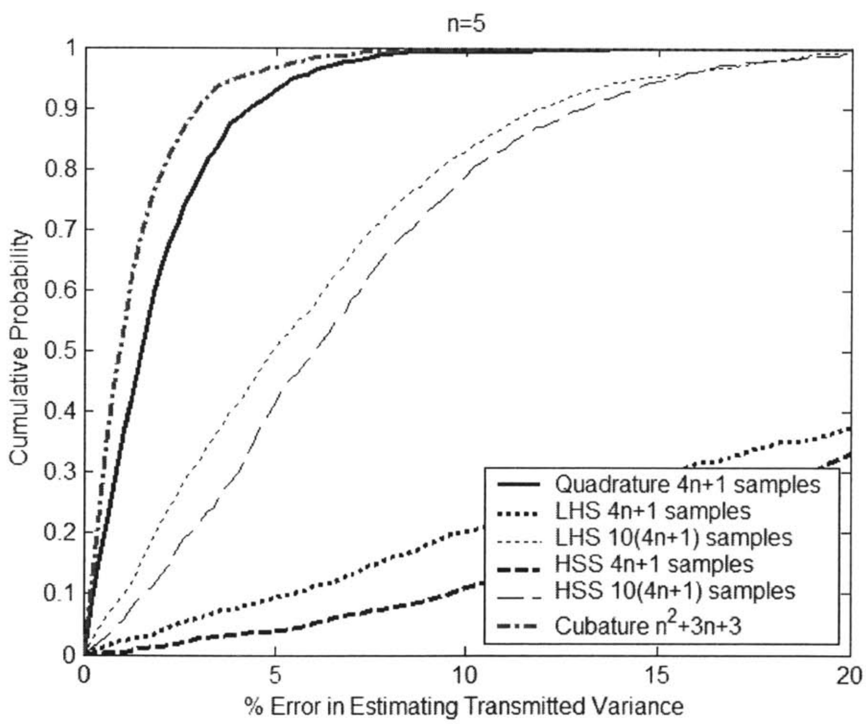


Figure A.2 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 5^{th} order polynomials of five inputs (n=5)

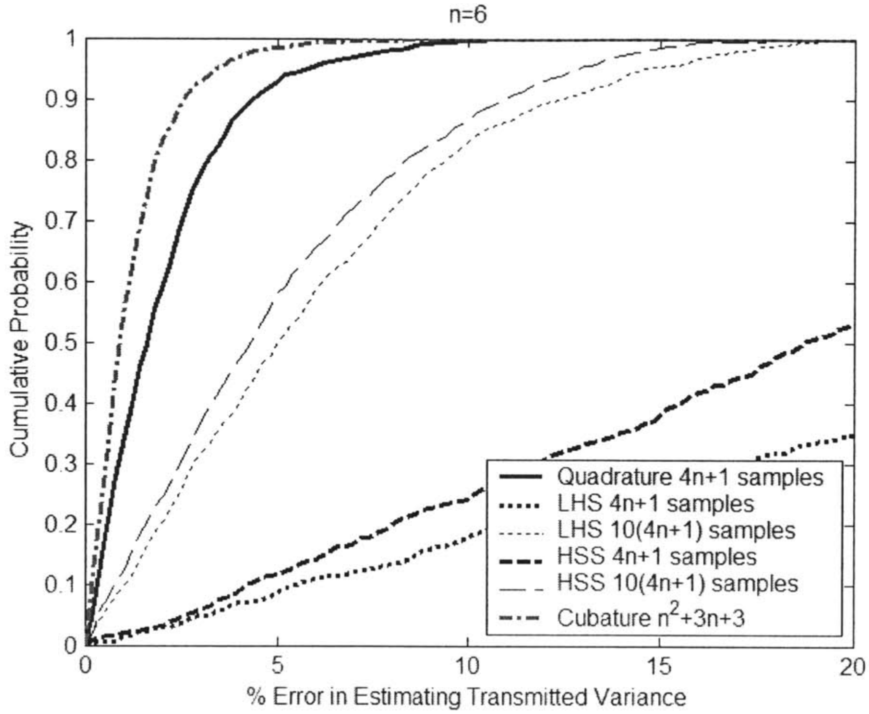


Figure A.3 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 5^{th} order polynomials of six inputs (*n*=6)

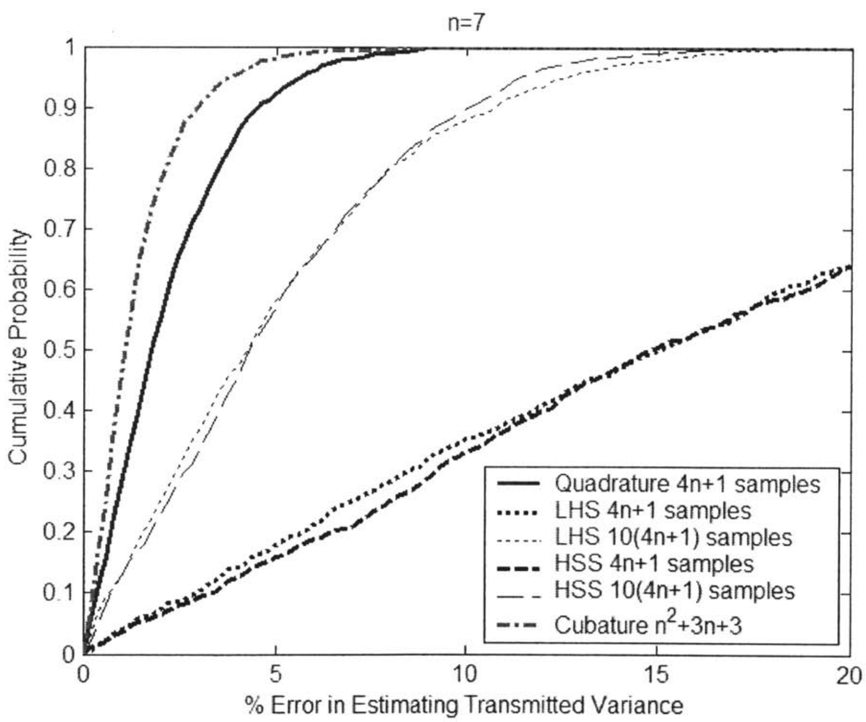


Figure A.4 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 5^{th} order polynomials of seven inputs (*n*=7)

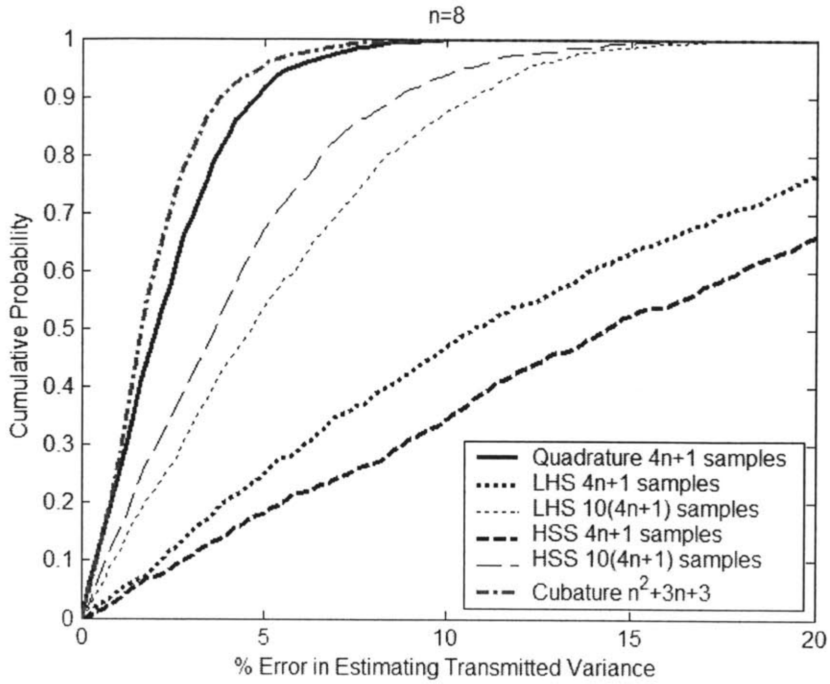


Figure A.5 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 5th order polynomials of eight inputs (n=8)

Appendix B: Cumulative probability versus relative error in estimating transmitted variance for the Third Order Hierarchical Probability Model (Equations B.1 to B.4).

Due to the computational burden in the fifth Order hierarchical probability model (Equations 4.11 to 4.16) when n>8, the following third order hierarchical probability model (Equations B.1 to B.4) are used to compare the accuracy of the quadrature-based method to alternatives when n=6~20. The third order model is obtained by simply letting β_{ijkl} and β_{ijklm} in Equation 4.11 to zero.

$$y(\mathbf{z}) = \beta_0 + \sum_{i=1}^{n} \beta_i \mathbf{z}_i + \sum_{j=1}^{n} \sum_{\substack{i=1 \\ i \le j}}^{n} \beta_{ij} \mathbf{z}_i \mathbf{z}_j + \sum_{k=1}^{n} \sum_{\substack{j=1 \\ j \le k}}^{n} \sum_{\substack{i=1 \\ i \le j}}^{n} \beta_{ijk} \mathbf{z}_i \mathbf{z}_j \mathbf{z}_k \tag{B.1}$$

where the independent variables are normally distributed random variables and the polynomial coefficients are also normally distributed and subject to geometric decay with increasing order.

$$\beta_i \sim N(0, \tau^2 r) \tag{B.2}$$

$$f(\beta_{ij}) = \begin{cases} N(0, \tau^2 r^2) & if \quad i = j \\ N(0, \tau^2 r_{INT}^2) & otherwise \end{cases} \tag{B.3}$$

$$f(\beta_{ijk}) = \begin{cases} N(0, \tau^2 r^3) & if \quad i = j = k \\ N(0, \tau^2 r_{INT}^3) & otherwise \end{cases} \tag{B.4}$$

A variety of alternative procedures applied to populations of 3rd order polynomials whose polynomial coefficients decrease geometrically with order at rate $\sqrt{r}$ =0.2 for single factor effects and at a faster rate ($\sqrt{r_{INT} / r} = 0.6$) for interaction effects. Each Figure is based on a population of 1,000 systems generated from the Hierarchical Probability Model (Equations 4.11 to 4.16).

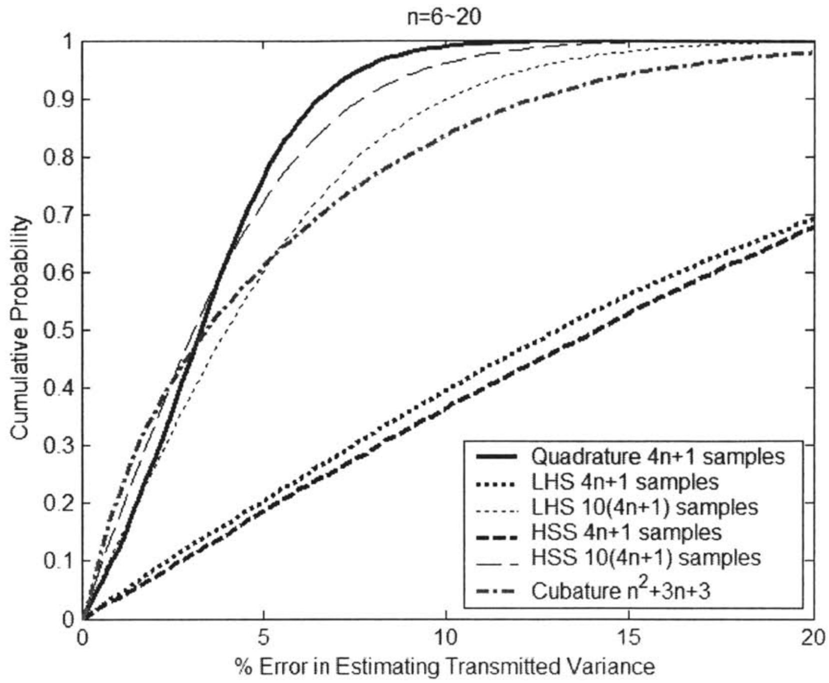


Figure B.1 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 15,000 systems of 3rd order polynomials of six inputs (n=6~20)

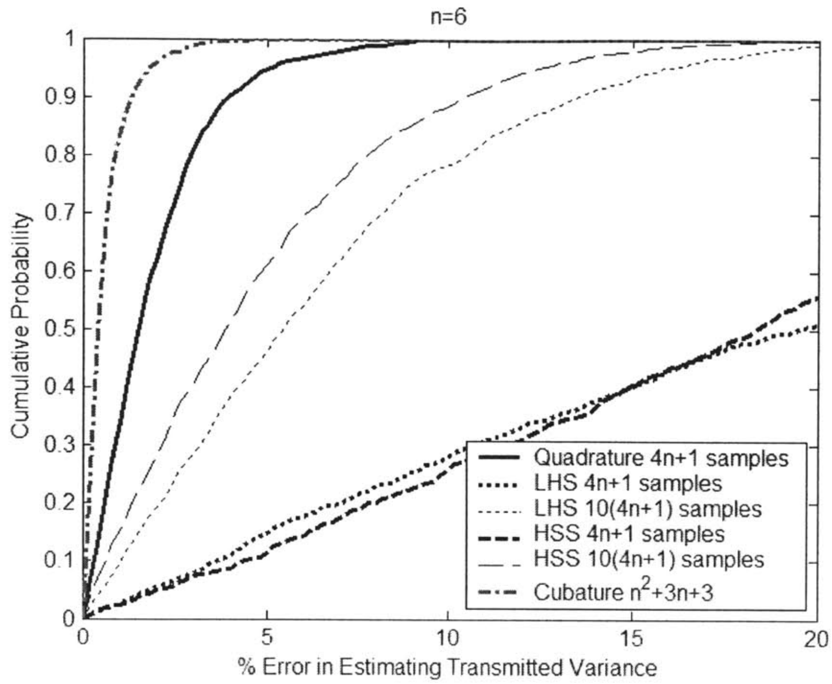


Figure B.2 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd order polynomials of six inputs (n=6)

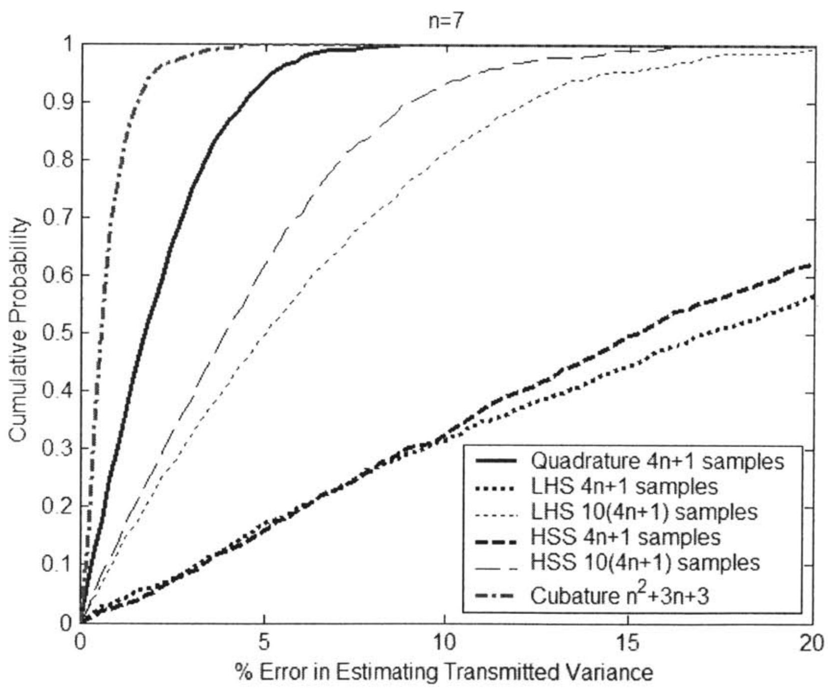


Figure B.3 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd h order polynomials of seven inputs (n=7)

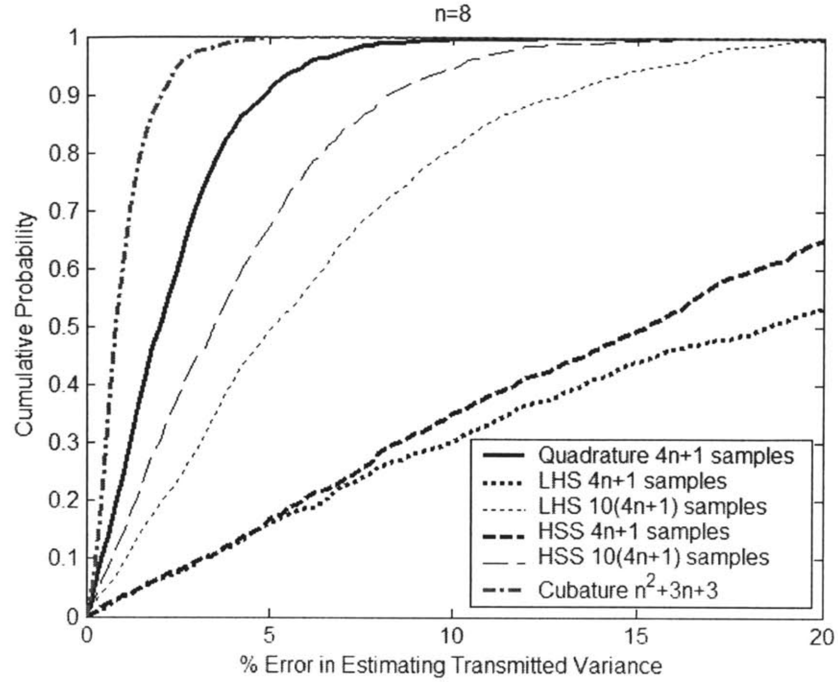


Figure B.4 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd order polynomials of eight inputs (n=8)

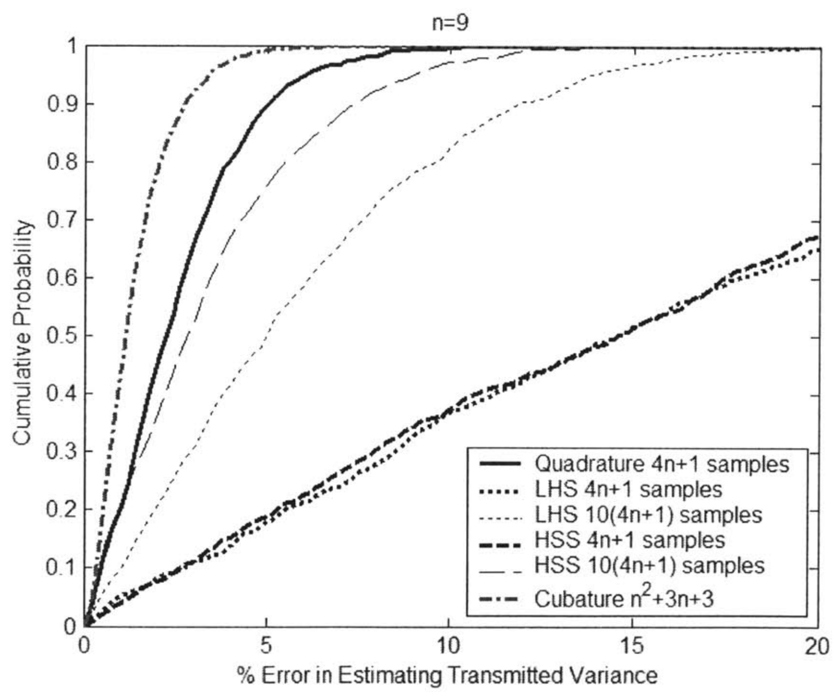


Figure B.5 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd order polynomials of nine inputs (n=9)

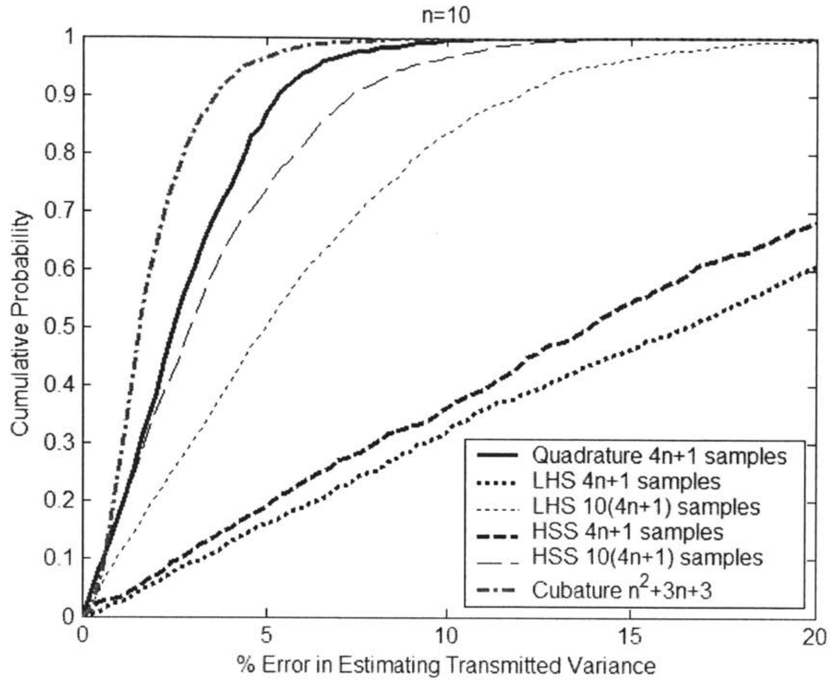


Figure B.6 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd order polynomials of ten inputs (n=10)

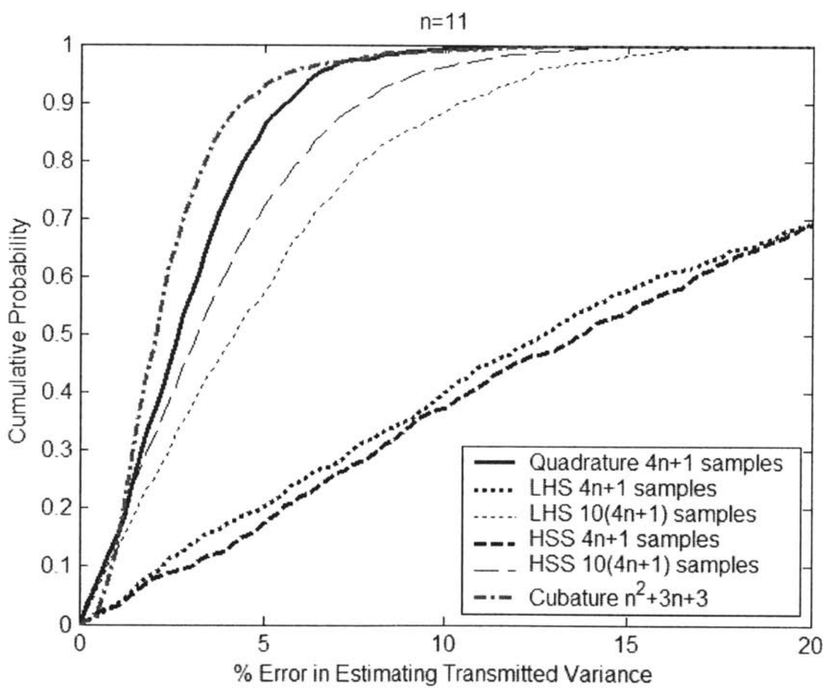


Figure B.7 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd order polynomials of eleven inputs (n=11)

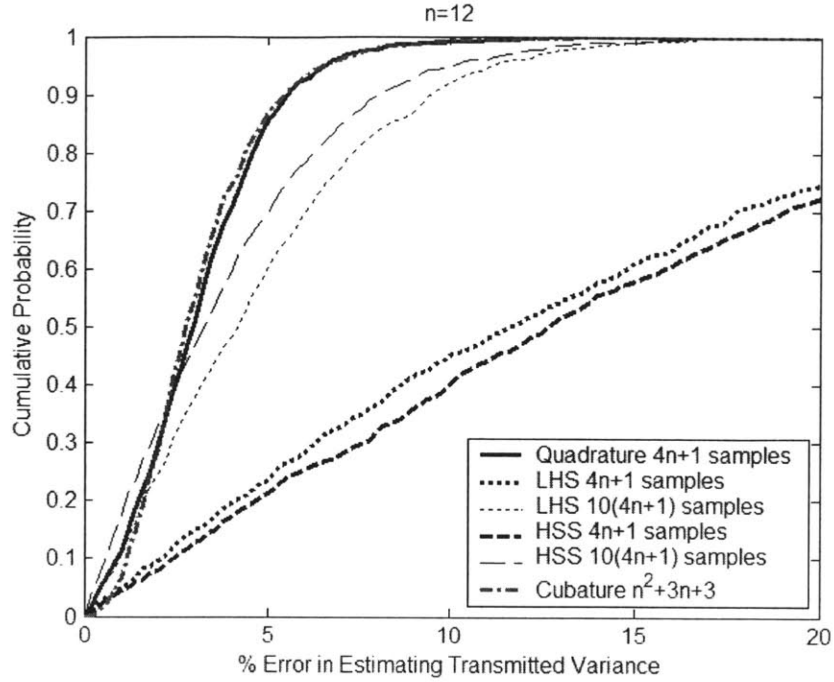


Figure B.8 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd h order polynomials of twelve inputs (n=12)

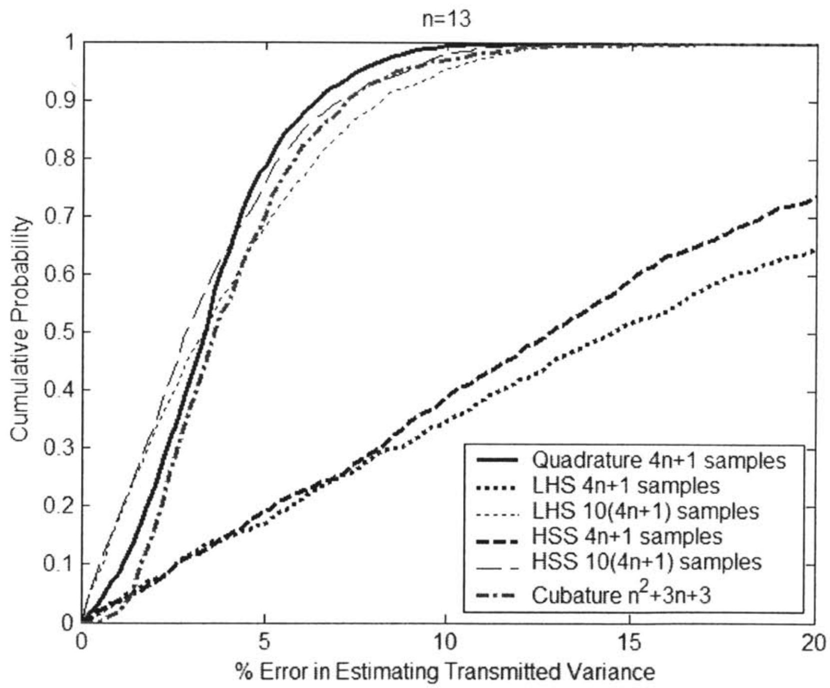


Figure B.9 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd order polynomials of thirteen inputs (n=13)

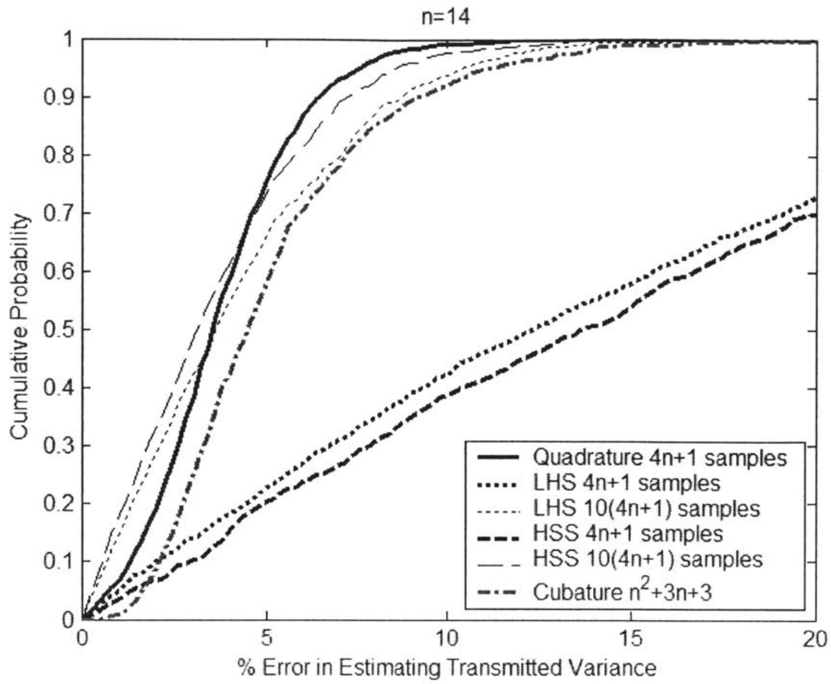


Figure B.10 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd order polynomials of fourteen inputs (*n*=14)

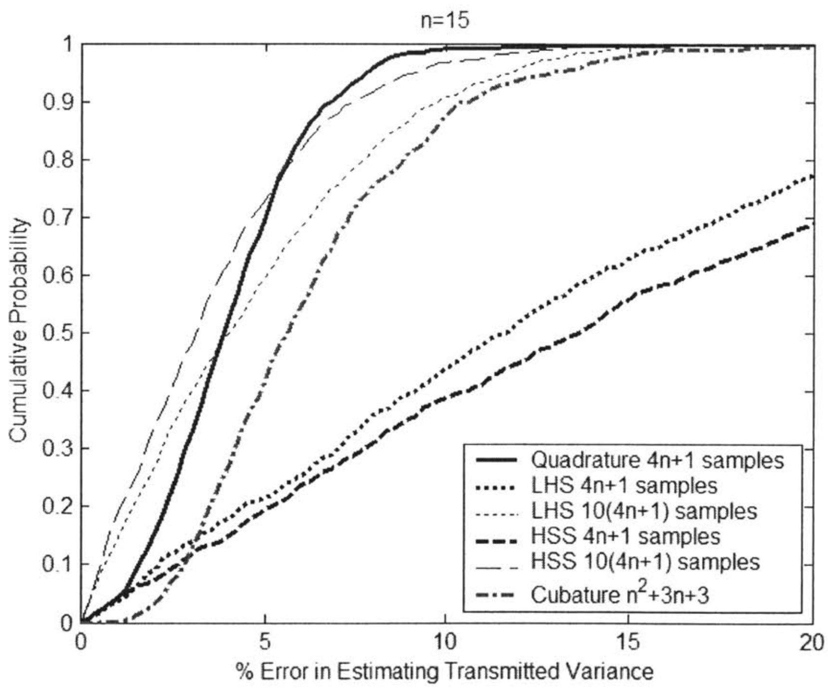


Figure B.11 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd order polynomials of fifteen inputs (*n*=15)

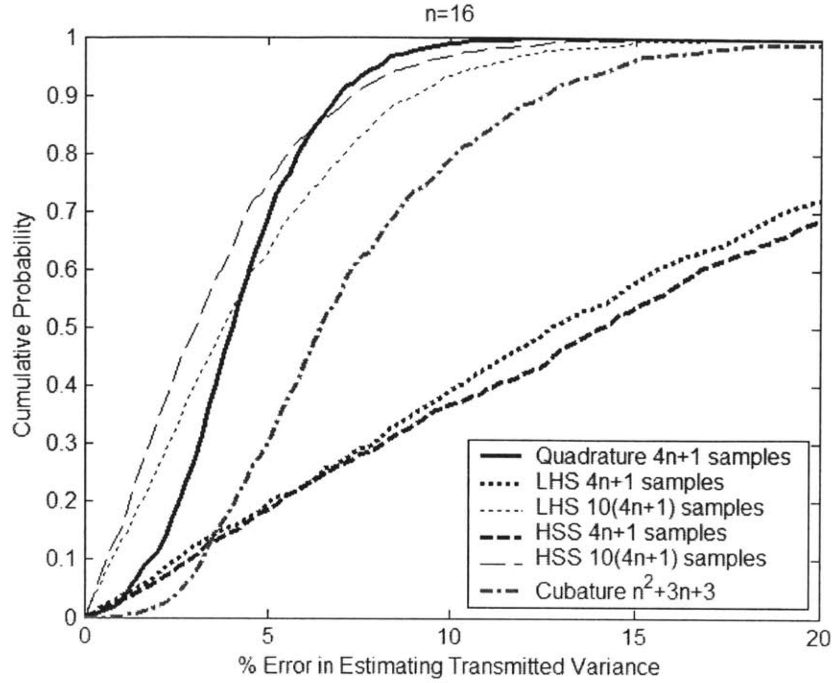


Figure B.12 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd order polynomials of sixteen inputs (n=16)

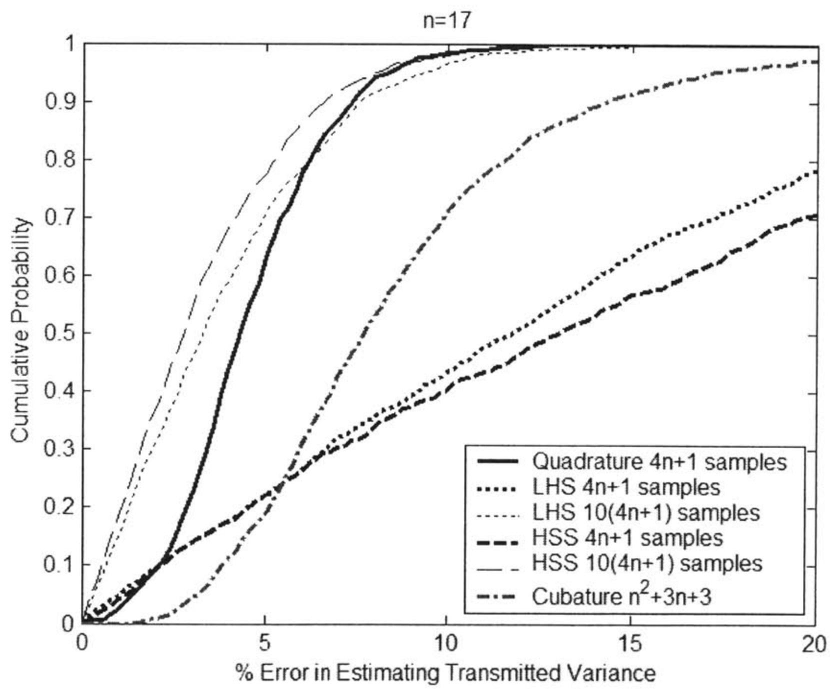


Figure B.13 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd h order polynomials of seventeen inputs (n=17)

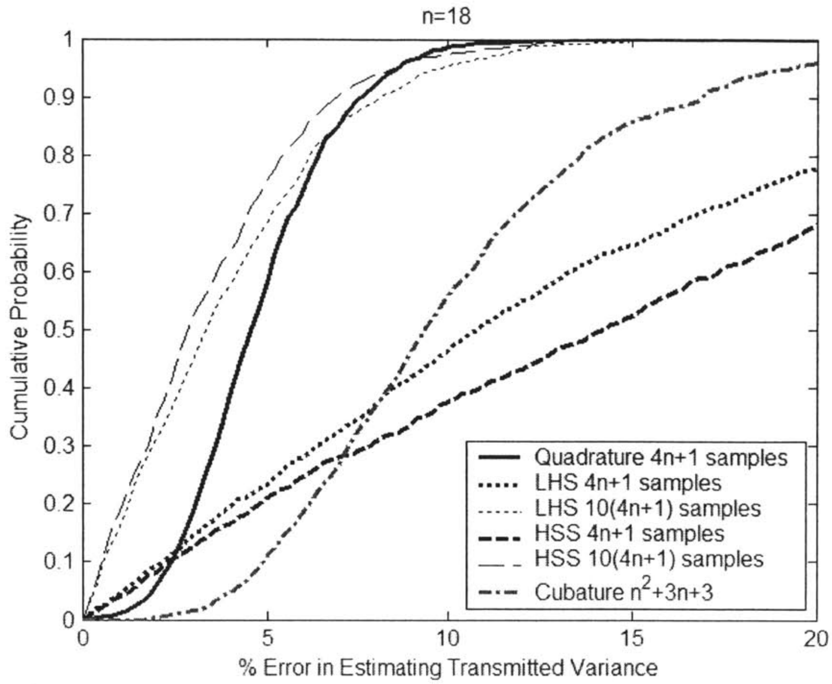


Figure B.14 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd order polynomials of eighteen inputs (*n*=18)

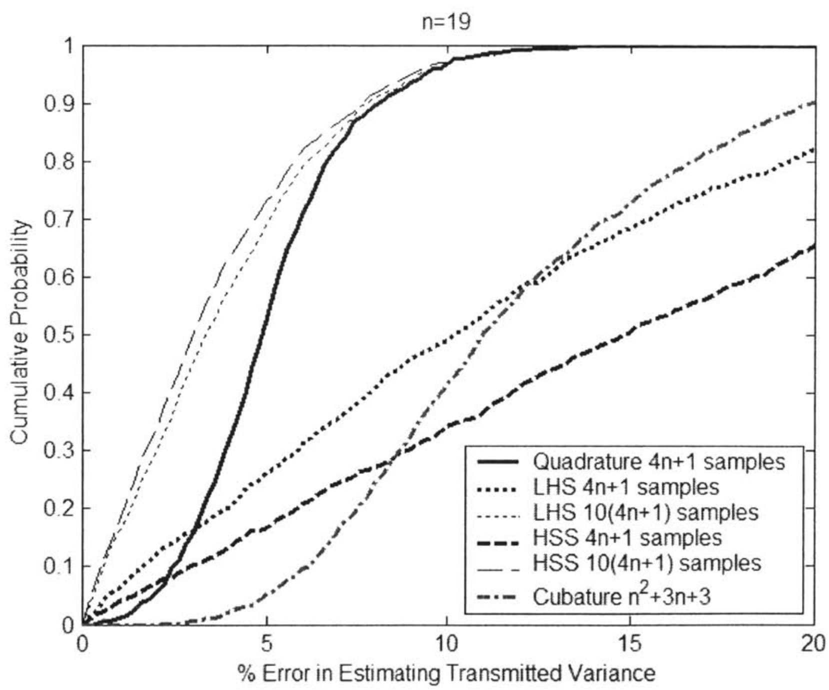


Figure B.15 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd order polynomials of nineteen inputs (*n*=19)

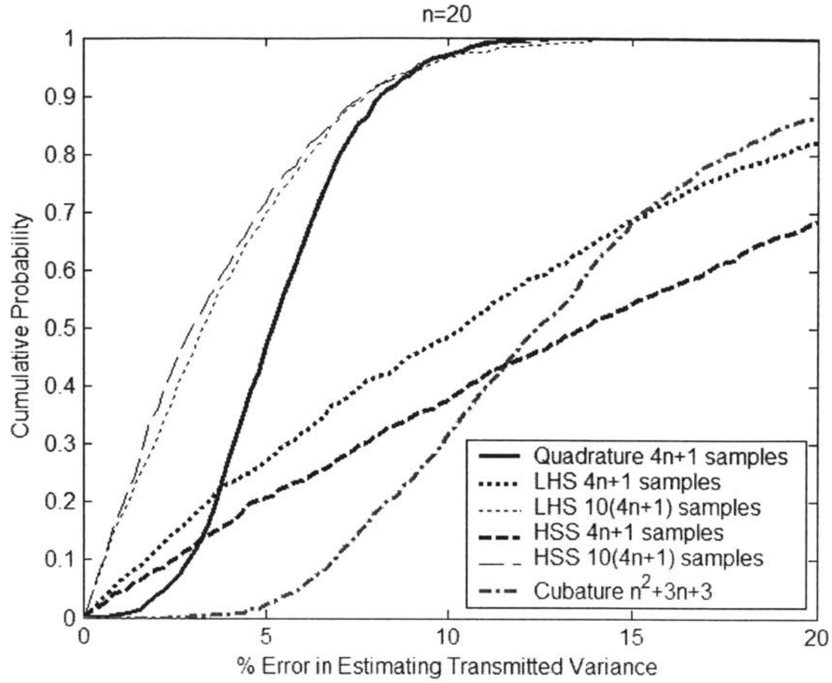


Figure B.16 Cumulative probability versus relative error in estimating transmitted variance for a variety of alternative procedures applied to 1000 systems of 3rd order polynomials of twenty inputs (n=20)

5112-37