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Robust Design Using an Efficient Sampling Technique

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Abstract

The concept of robust design involves identification of design settings that make the product performance less sensitive to the effects of seasonal and environmental variations. Batch processes are more flexible compared to continuous processes and are frequently used in these situations. Stochastic optimization methods provide a general approach to robust/ parameter design as compared to conventional techniques. However, the computational burden of these approaches can be extreme and depends on the sample size used for characterizing the parametric variations and uncertainties. In this paper, we present a novel sampling technique. The example of robust batch distillation column design illustrates that the new sampling technique offers significant computational savings and better accuracy.

Keywords: robust design, Off-line quality control, stochastic optimization, sampling techniques, batch distillation, Monte Carlo Methods.

1 Introduction

Robust/Parameter design is an off-line quality control method popularized by the Japanese quality expert G. Taguchi, for designing products and manufacturing processes that are robust in the face of uncontrollable variations (Bendell et al., 1990). At the design stage, the goal of parameter design is to identify design settings that make the product performance less sensitive to the effects of manufacturing and environmental variations, and deterioration.

The most general approach to the robust or parameter design problem is to couple an optimizer directly with the computer simulation model using stochastic descriptions of the noise factors (Boudriga, 1990; Diwekar and Rubin, 1994). These general class of problems can be characterized as stochastic optimization problems. The stochastic optimization problem involves the evaluation of an aggregate measure (used as a performance statistics) derived from a multivariate probability distribution. For nonlinear models, this is done numerically using a representative sample from the multivariate space and has to be repeated at each optimization iteration. Therefore, an efficient sampling scheme which reduces the number of samples required for each iteration can significantly improve the computational efficacy of the stochastic optimization procedure.

In this paper, we present a new and efficient sampling technique using the shifted Hammersley points for uniformly sampling a k-dimensional unit hypercube. This new sampling techniques requires far fewer samples as compared to other techniques to approximate the mean and variance of distributions derived by propagating a representative sample (for the inputs) over nonlinear functions. For the robust design problem posed in terms of stochastic optimization, the use of this efficient sampling technique can significantly alleviate the computational burden. We illustrate this in the context of robust design of a batch distillation column which is subject to feedstock variations, modeling uncertainties and measurement errors and report computational savings of upto a factor of 10.

2 Monte Carlo and Latin Hypercube Sampling Techniques

Perhaps one of the best known methods for sampling a probability distribution is the Monte-Carlo sampling technique which based on the use of a pseudo random number generator to approximate a uniform distribution, U(0,1) with n samples. The specific values for each input variables are selected by inverting the n samples over the cumulative distribution function. A Monte Carlo sample has the property that successive points are independent. However, in most applications, the actual relationship between successive points in a sample has no physical significance, hence the independence/randomness of a sample for approximating a uniform distribution is not critical (Knuth, 1973). Moreover, the error of approximating a distribution by a finite sample depends on the equidistribution properties of the sample used for U(0,1) rather than it's randomness. Once it is apparent that the uniformity properties are central to the design of sampling techniques, constrained or stratified sampling becomes appealing (Morgan and Henrion, 1990).

Latin Hypercube Sampling (LHS) is one form of stratified sampling which can yield more precise estimates of the distribution function (Iman and Shortencarier, 1984). The range of each u_i is divided into non overlapping intervals of equal probability. One value from each interval is selected randomly with respect to the probability density in the interval. The n values thus obtained for u_i are paired in a random manner with the n values of X_2 and these n pairs are combined with n values of X_3 and so on to form n k-tuplets. The random pairing is based on a pseudo random number generator. The main shortcoming with this stratification scheme is that it is one dimensional and does not provide good uniformity properties on a k-dimensional unit hypercube. Until recently, the only known design for uniformity on a d-dimensional hypercube was a uniform grid (Papageoriou and Wasilkowski, 1990). However, the uniform grid requires exponential sample points in the number of variables for good equidistribution properties. This paper presents a new sampling technique which uses a quasi-random generator based on shifted Hammersley sequences. The shifted Hammersley sequences were shown to be a minimum discrepancy design by Wozniakowski (1991). This new sampling technique shows superior convergence properties.

3 The New Sampling Technique

Since most of the stochastic optimization problems involve integrals of some probabilistic functional, consider the approximation of an integral of a k-dimensional continuous function by sampling its values at a finite set of points. For sake of simplicity let us assume that the integration is restricted to a k-dimensional unit cube. One straightforward approach is to place the points along equally spaced intervals on a d-dimensional grid. Although this is a good arrangement, the number of points needed to keep the average error less than ϵ is roughly proportional to $\frac{1}{\epsilon^k}$. The traditional alternative is to use a Monte Carlo method where the points are chosen completely randomly using a pseudo-random number generator. The approximation to the integral is then based on the function evaluation at these points. Although on the average, the number of points required to keep the error within ϵ is bound by $\frac{1}{\epsilon^2}$ there is no methodical way for constructing the sample points to achieve the bound (Papageoriou and Wasilkowski, 1990).

In this section we describe a new sampling technique based on the use of the shifted Hammersley points. We call this new technique – the Shifted-Hammersley Sampling (SHS) technique. The basic idea behind this technique is to replace a Monte Carlo integration by a quasi-Monte Carlo scheme. The choice of an appropriate quasi-Monte

Carlo sequence is based on the concept of discrepancy. Discrepancy is a quantitative measure for the deviation of the sequence from uniform distribution. Therefore it is typically desirable to choose a low discrepancy sequence. Some examples of low discrepancy sequences are the Halton and Hammersley sequences. Without embarking on a detailed discussion of these issues (the interested reader is referred to Niederreiter (1992), it is apparent that we are faced with the issue of which sequence should one use for the design of a quasi-Monte Carlo sampling technique. The shifted Hammersley sequence has been shown (Wozniakowski 1991) to have the minimum discrepancy for the class of real continuous functions in the average case setting.

We provide a comparison of the performance of the Shifted Hammersley sampling (SHS) technique to that of Latin Hypercube (LHS) and Monte Carlo (MCS) techniques. The comparison is performed by propagating samples derived from each of the techniques for a set of n-input variables (X_i), through various nonlinear functions ($Y = f(X_1, X_2, ..., X_n)$) and measuring the number of samples required to converge to the mean and variance of the derived distribution for Y. Since there are no analytic approaches (for stratified designs) to calculate the number of samples required for convergence, we have conducted a large matrix of numerical tests. The design of the test matrix included varying of the type of function, the number of input variables, X_i, type of input distribution, and the correlation structures between them. The details of the test matrix are described below. A total of four sampling techniques have been compared: Monte Carlo, random Latin Hypercube, median Latin Hypercube, and the shifted Hammersley. The number of input variables used was varied between 2 and 10. Five different kinds of functions were used including 1) linear additive function, 2) multiplicative, 3)quadratic, 4) exponential, and 5) logarithmic. Three types of distributions have been used for the input variables X_i. Two of them, uniform and normal are symmetric and the the third is a skewed distribution, Lognormal. Three types of correlation structures have been used: the first is a zero correlation, and the other two sets use a correlation of 0.5 and 0.9 between the input variables. This matrix represents a total of 180 data sets (4 sampling techniques $\times$ 3 types of distributions $\times$ 3 correlation structures $\times$ 5 functions) for each set of input variables, X_i. As the number of input variables is varied from 2 to 10, it adds another factor of 9, i.e. 1620 data sets. However, in the interests of space and clarity we will present only the results which highlight the main findings of this numerical experiment. It has been established in the literature that LHS performs significantly better than MCS. The numerical experiments supported this result. Furthermore, it has been found that the SHS sampling technique has a much faster convergence rate as compared to LHS, anywhere from a factor of 1.5 to 100 and larger! For more discussion on the sampling technique and comparisons, please refer to Kalagnanam and Diwekar (1995).

4 Robust Design of a Batch Distillation Column

Batch distillation is an important unit operation frequently used for small-scale production. Batch distillation is preferable to continuous distillation when small quantities of high technology/high-value-added chemicals and biochemicals need to be separated. The most outstanding feature of batch distillation is its flexibility. This flexibility allows one to deal with uncertainties in feed stock or product specification (Diwekar, 1995). Therefore the concept of robust design is particularly relevant to batch distillation.

The sudden increase in the production of high value-added, low-volume specialty chemicals and biochemicals in recent years has generated renewed interest in batch distillation design. However, the current design procedures are still based on deterministic framework. We first present a description of the robust design problem in the context of batch distillation column design and then outline the sample size required to characterize the variance of the output

Table 1: PARAMETERS AND THEIR VALUES USED IN THE STUDY

Parameter	Values	Units	$E_i\%$
α	2.0		5
x_F	0.5	$mole\ fraction$	10
R	2.5		5
V	100	mol/hr	5
F	100	mol	10
x_D^*	0.95	$mole\ fraction$	
D_{spec}	36	$mole$	

from the process that needs to be controlled for quality. Finally, we present the computational burden of solving the robust design problem for both the sampling techniques.

For simplicity, consider a binary mixture with the feed composition of more volatile component to be x_F (mole fraction) and total feed F (moles) to be separated in a batch distillation column. There are variabilities and fluctuations in feed composition and feed amount over different batches which amounts to saying that the feed composition (x_F) and feed (F) are uncertain quantities. There are measurement errors in quantities like vapor boilup rate V (function of heat input to the reboiler), and reflux ratio R. The thermodynamic errors lead to uncertainties in relative volatility (α) predictions. Given the above variabilities and uncertainties we want to design a batch column which will maintain the amount of product with the given purity. These variations are assumed to be at $E_i\%$ error levels in the inputs, $E_i = \sigma_i/\mu_i \times 100$ normally distributed. Numerical values of the design and noise variables (nominal values, μ_i and % error levels E_i) are given in Table 1. So the problem of robust design translates into finding the number of theoretical plates and reflux ratio required to minimize the variance in the distillate amount of specific purity x_D*.

The iterative nature of the robust design calls for use of simplified models. The shortcut method presented by Diwekar and Madhavan (1991) provides an efficient alternative for robust design. Apart from computational efficiency, lower memory requirements, and the algebraic equation oriented form of the shortcut method, it is also useful in identifying feasible region of operation crucial for design problems. Furthermore, the dimensionality of the problem does not increase with increasing number of plates and the design variable number of theoretical plates is not an integer. These attributes makes the shortcut method desirable for robust design procedures. The robust design problem involves solution of a stochastic optimization problem where the optimizer in the outer loop finds the decision variables, number of plates N and reflux ratio R and the inner loop is the stochastic model. The shortcut method provides feasibility considerations which are used in this iterative procedure. The optimizer minimizes the error variance of the error in distillate amount collected and the specified distillate amount D_{spec}.

Since the objective from a robust design perspective is to minimize the variance in the amount of distillate, we characterize the number of samples required to estimate the variance to within 1% of its value using both Latin Hypercube and Shifted Hammersley points. The Shifted Hammersley points requires about 650 points to converge as compared to 6550 points required by the Latin Hypercube Sample. Figure 1a plots the variance as a function of number of samples. Figure 1b shows the variation in the product amount before and after the robust design, where the variance is reduced from 364 to 108 by changing the theoretical number of plates from 10.95 to 20.88 and reflux ratio from 2.5 to 3.0. This variance reduction at the expense of overdesigning is worthwhile when the product is valuable

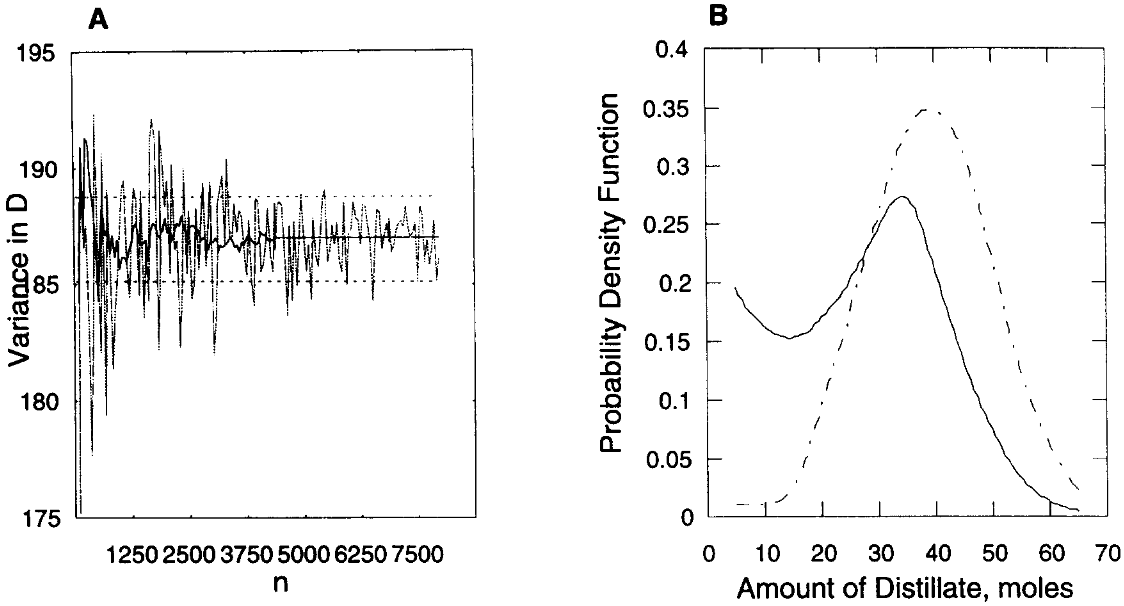

Figure 1: (a)Variance of error in D using LHS (dotted line) and SHS (solid line). 1% error band is shown by broken lines; (b) Variations in the amount of distillate, before (solid line) and after (broken line) design for quality

(given that designs which can give very small amount of product are avoided). The variance can be further reduced by Taguchi's tolerance design method.

5 Conclusions

This paper presented a new sampling technique based on shifted Hammersley points. This new sampling technique is shown to have better uniformity properties which reduces the computational intensity of stochastic optimization problem considerably. A robust design concept was introduced in the context of batch distillation column design operating under internal and external uncertainties. Since the robust design concept essentially involves solution of stochastic optimization problem, it was found that this sampling technique is always preferable for robust/parameter design problems. This is because of its high precision and consistent behavior coupled with great computational efficiency.

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