1. TAGUCHI ANALYSIS

1.1 Background

The principles of Dr. Genichi Taguchi's Quality Engineering, or Taguchi Methods, as they are often called in the United States, have had a dramatic impact on U.S. industry, particularly since the early 1980's, as more and more companies have started various programs and training methods with the hope of achieving some of the successes that various Japanese companies have experienced over the last thirty or more years. Case studies detailing successes at the Ina Seito Tile Co., the Electrical Communication Laboratory (Japan), the Kawasaki Oil Refinery, as well as seven other examples are given in (Taguchi) [130]. Many consultants travel throughout the U.S. presenting seminars and training workshops concerned with the learning and implementation of Taguchi methods, tools and applications. Taguchi methods have been used in such situations as VLSI circuit design (Welch *et al*) [142], non-destructive testing (McEwan, Belavendram, and Abou-Ali) [93], robot process capability (Black and Jiang) [14], thickness of aluminum deposits on silicon wafers (Aceves, Hernandez, and Murphy) [2], injection molded plastic components (Hanrahan and Baltus) [63], as well as cruise control vacuum valves, shrinkage of speedometer cable, computer response time, powers supply circuits, noise reduction in hydraulic rollers, and in reducing the rework rate of diesel injectors (Wu) [143]. More examples may be found in (Dehned) [37]. The American Supplier Institute holds an annual symposium devoted solely to Taguchi Methods, with the first held in 1983.

In most quality or quality control situations, the goal is to produce output as uniformly near a target value as possible. The reduction of variation is now regarded as a fundamental concept, both for those concerned with manufacturing and production and also for those focused on service or task processing. The Taguchi method is aimed at the manufacturing situation.

To understand the workings of Taguchi methods one must consider three possible situations concerning a quality characteristic of interest. These three are: larger values are better, smaller values are better, target value is best. A quality characteristic is an important dimension, property or attribute of a manufactured output. The three cases will be considered separately.

For the case where a target value is best, the aim of Taguchi methods is twofold: center some measured quality characteristic around a target value, and minimize the variation around this target value. The famous Sony-USA compared with Sony-Japan example illustrates that being centered at the target value is not enough, that being correctly centered at the target and being within specification limits is better, but the best situation is one of being centered at the target *and* having minimal variation around that target. (See Sullivan, [124]).

The realization that *both* the average output and the variability of the output are crucial is a tremendous improvement over the traditional engineering practice of only considering whether or not a part falls within specification limits. With regard to the implementation of (not the concept of) this idea, Taguchi has exerted a broad influence and deserves much praise. Any deviation from the optimal value is considered bad, the severity of the deviation is usually measured by a quadratic loss function. The loss to the manufacturer or society is considered to be proportional to the *square* of the distance from the optimal value. Mathematically, this loss can be written: $l(Y) = k(Y - T)^2$, where Y is the observed value and T is the optimal or target value. The constant, k, can be determined based on the loss at a fixed value of $Y - T$. This fixed value may represent the edge of the specification limits, or might be a point at which it is felt that, say, 50% of the customers would complain or require warranty work. The squared error loss is motivated by a Taylor series expansion. (See Taguchi, [129] and [130]). Minimizing this loss (or expected loss) is consistent with the two goals of the Taguchi Method. The squared error loss function is a continuous function, and is strictly increasing in $|Y - T|$, as opposed to the discrete pass/fail nature of specification limits. This loss function is also effective in convincing people to worry about variation even when the process is on target and may even be within the desired specification limits. In particular, if the loss is expressed in dollar units, those at the management level will now be more concerned about reducing variation.

Consider next the situation where smaller values are better, but the response or quality characteristic of interest is non-negative. In this situation we are concerned with the same loss, $k(Y - T)^2$, except now we set the target value to zero and hope to minimize $E(Y^2)$, which represents the mean squared error, or mse, around zero.

The final situation is that in which the response is again non-negative, but here larger values are considered to be better. The goal is to maximize $E(Y^2)$. Here the Taguchi practitioner considers $E(1/Y^2)$ and again tries to minimize this quantity. The quantities to be minimized stem from the desire to measure and reduce the variation relative to the target value. However, the Taguchi method does not base its analysis directly on the above quantities; the exact quantity to be optimized for each of these three situations will be given later. In using the reciprocal squared as the quantity of interest, the larger is better situation now becomes that of smaller values being better, and we proceed as in the smaller is better situation.

The first step in implementing the Taguchi Method is that of parameter design. Parameters are various inputs suspected or known to have an effect on the quality characteristic, and might include such things as rate of flow, temperature, humidity or reaction time. Parameter design is an investigation to determine which variables or parameters have an effect on the quality characteristic. This attempts to improve on quality while still at the design stage, as opposed to intensive sampling plans that inspect their way to high quality by 'catching' poor output. Designing high quality and low variability into the product will not only be much cheaper than extensive or exhaustive inspection, but also will allow a product to go from blueprint to usable product in much less time. Variables suspected to have some effect on the quality characteristic of interest are known as factors. At this point any expert knowledge of the subject matter should be applied in the selection of variables to include as factors. Those variables suspected to have the largest effects on the quality characteristic are generally considered first but it is very possible to (unknowingly) omit variables that should have been considered and also to include others that have no effect on the quality characteristic. Once chosen, these variables are then classified into one of two categories: control variables or noise variables. Control variables represent those parameters or factors which can be controlled by the designer or manufacturer. In contrast, noise variables are those parameters which may have an effect on the quality characteristic but generally cannot be controlled by the designer. Variables that are very expensive or very difficult to control may also be considered noise variables.

In order to screen these variables for their effect on the quality characteristic, a classical Taguchi designed experiment takes place. Various settings are selected for each of the control variables and various settings are *temporarily* fixed for each of the noise variables. The controllable factors are placed into what is known as the *inner array.* The inner array is somewhat similar to the classical 'design matrix'. Each row of this inner array represents one particular combination of settings for the control factors, or one 'design point'. Thus an inner array with eight rows represents eight possible configurations of the control factors. The noise factors are placed into what is termed the *outer array.* The settings for the outer array should represent a range of possible noise conditions that will be encountered in everyday production, although in practice it is very common to consider only two or three levels for each of the control factors. Again, these settings are fixed solely for the purpose of the experiment, in general they will be random. If the noise is assumed to have a linear effect, the two settings would generally be $\mu_{noise} \pm \sigma_{noise}$, when the noise factor is suspected (or known) to have a quadratic effect on the quality characteristic, the (three) settings would generally be $\mu_{noise} - \sqrt{3/2}\sigma, \mu_{noise}, \mu_{noise} + \sqrt{3/2}\sigma$. "These choices are apparently based on the assumption that the noise factors have approximately symmetric distributions" (Kackar, [78]). The two arrays are then *crossed*, which means that every experimental condition called for by the inner array of control factors takes place at every condition called for by the outer array of noise factors. In this way all of the points in the inner array are exposed to the same values of the noise factors in the outer array; it is hoped that the temporarily fixed settings of the noise factors at the experimentation level will approximate the random conditions that will occur at the production level. Data measurements on the quality characteristic of interest are then collected. In some cases the quality characteristic will be obvious: final weight of an expensive product sold by weight, diameter of a cylinder, length of a shaft, shipping weight of a box of cereal, number of defective welds on an assembly, time to complete a crucial task, purity of a final product, number of blemishes on a car door, number of cycles until failure of a key mechanical part, or the amount of stress before failure of a cable or attaching mechanism. The question of what to measure is best answered by a person with expert knowledge in the area, not by an expert in Taguchi methods or in statistical analysis. Particularly in the engineering sciences, any knowledge of the underlying physical structure should be used as an aid in choosing which variables to include in the design, and also in determining what quality characteristic should be measured. This subject matter knowledge may also serve to point out what ranges of these variables should be considered, ranges that may or may not coincide with the ranges of the 'knobs' that can be turned. Moreover, subject matter knowledge may serve to point out that the control variables or 'knobs' available represent some transformation of the underlying variables that drive the process or reaction. An example of this would be where the quality characteristic depends critically on the density of a mixture, but the 'knob' available to the experimenter is blending speed.

In general, for an inner array with m settings of the control factors and n configurations of the noise variables, the Taguchi method requires mn observations, even more if there are replications. The two arrays are most often balanced, which means that for any column of either array, an equal number of observations are taken for each setting that is given in the array. Furthermore, for any pair of columns (from the same array), any combinations of factors that do occur will occur the same number of times. Thus if the setting where factor A is at level one and factor B is at level three occurs four times in the inner array, then *any* combination of factors A and B that does occur must occur exactly four times in the inner array. The arrays are generally also orthogonal, which means that the vector product $\underset{\sim}{x}_i'\underset{\sim}{x}_j$ is zero if $i \neq j$, where $\underset{\sim}{x}_i$ and $\underset{\sim}{x}_j$ represent columns from the same array, suitably scaled, centered at zero. This balance in the arrays allows the experimenter to determine the effects of individual factors by averaging over the levels of the other factors. The data collected consist of measurements of some quality characteristic, collected at each setting dictated by the two crossed arrays. This characteristic might be, for example, percent purity, yield, or length of some critical dimension. Controllable factors to be placed into the inner array might include engine speed, amount of a certain chemical, thickness of a metal part, amount of adhesive applied, voltage through a resistor, gas flow, mixing speed, spring tension, initial load etc. These represent variables that can easily and effectively be controlled by the experimenter or manufacturer. Noise factors in the outer array could include ambient humidity in a large factory, a particular lot or batch of a key ingredient, cleanliness of a part, the supplier of a key input, or amount of time since last lubrication. The noise variables and control variables to be included in any experiment tend to be particular to the situation being considered; those most familiar with the output of interest will often have a general idea of what forces, controllable or otherwise, have an influence on the output of interest.

The inner array is sometimes referred to as the design space, while the outer array is sometimes referred to as the environment space. The settings in each of the arrays generally represent a factorial design or a fractional factorial design. A factorial design is one where every value or level of each factor occurs with all levels of every other factor. Consider an inner array with three factors. If one factor has two levels, one has three levels and one has four, a factorial design (for this array) would require $2*3*4 = 24$ observations, more if replications are desired. This inner array would then be crossed with the outer array, requiring even more observations. A fractional factorial design is a design that considers only some carefully selected

Table 1.1 Taguchi Crossed Arrays, 32 observations

	$z_1 = 1$ $z_2 = 1$	$z_1 = 1$ $z_2 = 2$	$z_1 = 2$ $z_2 = 1$	$z_1 = 2$ $z_2 = 2$
x_1	1 1 1 1 2 2 2 2	1 1 1 1 2 2 2 2	1 1 1 1 2 2 2 2	1 1 1 1 2 2 2 2
x_2	1 1 2 2 1 1 2 2	1 1 2 2 1 1 2 2	1 1 2 2 1 1 2 2	1 1 2 2 1 1 2 2
x_3	1 2 1 2 1 2 1 2	1 2 1 2 1 2 1 2	1 2 1 2 1 2 1 2	1 2 1 2 1 2 1 2
#	$1, 2, \ldots$	$9, 10, \ldots$	$17, 18, \ldots$	$25, 26, \ldots$

fraction or portion of a factorial design. Typically two or three settings are considered for each of the variables, and a fractional factorial design would reduce the number of observations required by powers of 1/2 or powers of 1/3, by running, say, only one half or one ninth of the possible design points required for the factorial design. The design points actually chosen for the fractional factorial design usually, under certain conditions, maintain the orthogonality and balance of the full design. Such designs can often provide sufficient information while saving time and money. For example, imagine five design variables, each with two levels. These could be placed into a 2^{5-2} fractional factorial design, which is a $\frac{1}{4}$ fraction of a 2^5 experiment. The (full) factorial design calls for $2*2*2*2*2 = 32$ observations, while this quarter fraction calls for only eight. The outer array might then be a 2^3 design, which is an experiment having three (noise) factors, each at two levels. The two arrays, inner and outer, would then still be crossed, requiring 8∗8=64 runs. If constraints dictated that only 32 runs were possible, the experimenter might chose to run only one half of the 2^3 outer array,(2^{3-1}), giving a 50% savings in time and money. To illustrate the crossing of the two arrays, see table 1.1, where the following layout is presented. The inner array of the control factors, x_1, x_2, x_3, is a 2^3 design, crossed with a 2^2 outer array of noise factors, z_1 and z_2, and would require $32 = 8*4$ observations. In the Taguchi notation, this would be described as a $L_8(2^3)$ crossed with a $L_4(2^2)$. This may or may not be a layout recommended by Taguchi, it is included only to illustrate the crossing of the inner and outer arrays.

The Taguchi method includes the noise factors in the experiment for the purpose of identifying control factors settings which are robust against noise, i.e. those settings of the design factors which produce the smallest variation in the response across the different levels of the noise factors. Some combinations of control factor settings may yield output that is affected by the noise factors, thus causing the response to vary around its mean, while for others combinations the output is insensitive to the changes in the noise factors. (Phadke) [111]. Similarly, the quality characteristic might exhibit more variability at, say, the low setting of a certain control factor than it does at the high setting. For other control factors, the variation in the quality characteristic might be nearly constant across the levels of those control factors, while the average quality characteristic might or might not change across the levels of these control factors. For any control factor, there are four possible situations – effect or no effect on the mean, coupled with effect or no effect on the variation. If the experimenter is fortunate, some factors may arise that impact the mean but not the variation. Factors with this type of effect have been termed "performance measures independent of adjustment" or PerMIA - (Léon, Shoemaker, and Kackar) [88]. Such 'adjustment' factors may be used to move a process onto or towards its target value, without affecting the variation around the target. In a two-step adjustment process, the variation is minimized by the appropriate settings of the factors that affect the variation, and then the output is centered at the target value by the appropriate settings of the factors that only influence the mean. Factors which appear to have little or no impact on either the mean or the variation are typically set to the level representing the lowest cost.

In order to achieve its goals, the Taguchi method analyses not the measured response but rather some transformation of that response, depending on the situation. As mentioned previously, the Taguchi method aims to minimize the expected loss, $E(Y-T)^2$, but it does not base the analysis on this quantity directly. A signal to noise ratio is calculated, the choice of the particular signal to noise ratio depends on the desired outcome of the response: target or nominal is best, smaller is better, larger is better. The last two are considered equivalent by taking reciprocals. For all three situations, the analysis falls under Taguchi's idea of Signal to Noise ratio, although only in the target is best case are both signal and noise considered. (Taguchi is said to have coined the term 'signal to noise' in order that it appeal to the electrical engineers with which he was working during the 1950s - (Barker) [10]).

For the target is best situation, deviations from target in either direction must be considered. In order to minimize the $E(Y-T)^2$ the experimenter must be concerned with both variance and bias. In this situation Taguchi suggests that the following signal to noise ratio be considered: $10\log_{10}(\overline{y}^2/s^2)$, which is to be maximized. This ratio is calculated for each level of each control factor, averaging over the various noise levels, and over the other control factors. This ratio is also calculated for each 'design point', averaging over the settings of the noise factors in the inner array. It should be noted that maximizing this ratio is equivalent to maximizing $\overline{y}/s$, which is equivalent to minimizing the sample coefficient of variation, $s/\overline{y}$. In calculating this ratio, the Taguchi practitioner is simply performing a data transformation. For the larger is better situation the signal to noise ratio is $-10\log_{10}\frac{1}{n}\sum(1/y_i)^2$, for the smaller is better situation the signal to noise ratio is $-10\log_{10}\frac{1}{n}\sum y_i^2$. In all cases, the goal is to maximize the signal to noise ratio.

By analyzing the signal to noise ratio that is recommended for a particular situation, the Taguchi practitioner hopes to find which levels of design variables were insensitive to the variation in the noise variables, i.e. which setting in the inner array gave the smallest variation in response across the outer array. By constructing the same signal to noise ratio for each level of each control factor, across all other factors, the researcher may also discover that some factors affect the mean while others have an effect on the variation. Such factors are known as location effects and dispersion effects, respectively (Box and Meyer) [19].

As stated previously, the Taguchi method calls for this signal to noise ratio to be calculated for the data coming from each experimental setup of control factors. Thus this ratio is calculated for each row of the inner array. Based on the calculated signal to noise ratios, with higher being better, the 'best' levels of each of the control factors are assigned. For 'location effects', the signal to noise ratio allows the researcher to see the magnitude of the effect on the quality characteristic, measured across the levels of the noise factors. If the effect is small the experimenter may choose the control factor setting that represents the lowest cost. Mean plots may also be calculated for each of the levels of the control factors; the extent to which these agree with the signal to noise ratio plots will depend on the nature of the dependence between μ and σ. This graphical technique often accompanies the more classical technique of Analysis of Variance (ANOVA). Since the Taguchi design crosses the two arrays, it is possible to conduct an ANOVA on both the mean and the signal to noise ratio. Under the Taguchi system it is quite typical to verify the 'optimal' results with experimental follow-up.

Another approach (which may be impossible in some situations) is to first minimize the variation by picking the best levels of factors that affect only the variation, and the bring the process 'on target' by selecting the best levels of (other) factors that influence only the mean. The hope here is that the appropriate signal to noise ratio can be minimized in a two stage fashion. If the process target changes, the experimenter then only has to worry about one set of factors, since the other factors have been selected to minimize variation independently of the mean. In many applications of Taguchi methods, this partitioning of variables into disjoint categories based on whether they affect the mean or the variance is an assumption made before the data are collected. For a multiplicative error model, which says that the error increases in proportion to the mean, the maximization of the signal to noise ratio and the minimization of $E(Y-T)^2$ are equivalent. The Taguchi idea is to use a two-stage minimization procedure, first maximizing the signal to noise ratio over the factors that effect the variation, then adjusting the process to target by selecting the appropriate levels of those factors that effect the mean but not the variation. Under the assumption of a multiplicative error, we have $E(Y) = \mu, Var(Y) = \mu^2\sigma^2$, thus the mse is $(\mu - T)^2 + \mu^2\sigma^2$, and is minimized (over μ) at $\mu^* = T/(1+\sigma^2)$. The signal to noise ratio is $10\log_{10}((E(Y))^2/Var(Y))$, which can be written $10\ \log_{10} 1/\sigma^2$, and is to be maximized. Thus the variance could first be minimized (by maximizing the signal to noise ratio), and would have a minimum value, say σ_{min}. The other factors could be used to set the response at $\mu_{min} = T/(1+\sigma^2_{min})$. Therefore, maximizing the signal to noise ratio will be equivalent to minimizing the mse in a two step fashion. More information on the details of the two-stage minimization, the assumptions required and a comparison of signal to noise ratio against mse for various models are given in (Léon, Shoemaker, and Kackar) [88], as well as (Box) [21]. Note that in an additive model, $E(Y^2)= \sigma^2 + \mu^2$, and thus the signal to noise ratio for the smaller is better situation, $-10\log_{10}\frac{1}{n}\sum y_i^2$, clearly mixes together the effect on the mean and the effect on the variance.

A third approach (Vining and Myers) [139] is to set the mean at the appropriate level while at the same time minimizing the variance within the framework of a Response Surface model. Details concerning response surface methods (rsm) and models will be given in the following chapters. Within this context, the experimenter is concerned with both location and spread, and the mathematical modeling that takes places amounts to constrained optimization within the framework of a general linear model. For example, in the target is best situation this method calls for the experimenter to minimize σ^2 subject to the constraint $\mu = T$. For the other two cases (more extreme is better) the experimenter places the constraints on σ and optimizes μ subject to the various restrictions. Lagrange multipliers are then used to determine the optimal levels of the input factors. Quite often, however, an improvement in mean response will be accompanied by increased variation, and thus the final choice of design settings will often represent a tradeoff between minimum variance and minimum bias. Contour graphs for both the mean and the standard deviation are very useful in determining what settings represent the best choice. The approach given by these authors amounts to modeling both the mean and the variance but does not suggest how noise variables could be incorporated into the analysis.

1.2 Potential Flaws

Within the statistical community the acceptance and implementation of so called 'Taguchi-Methods' has not matched the optimism of industry. Many statisticians see a lot of good things within the Taguchi framework but point out many shortcomings as well. For a discussion involving both schools of thought, see (Barker *et al*) [9], as well as (Pignatiello and Ramberg) [112].

Although fractional factorial designs can provide a great deal of information with small to moderate sample sizes, the crossing of the two arrays in the Taguchi design often requires that a large number of observations be taken, with more observations almost always meaning more time and greater cost. This may be particularly bad if the experiment is of the 'screening' type, where a large number of factors, both noise and control, are being considered. The large number of runs called for by the crossed inner and outer arrays is one of the frequent criticisms of the Taguchi method.

Furthermore, there are those in the statistical community who view this crossing of the arrays as inefficient in terms of information (loss of information). Because the two arrays are crossed, the overall resolution of the design may not be as high as it could be with a different design. In many cases, this crossing results in the inability to handle or estimate significant interactions. Some suggest combining the two types of factors into a single combined array, i.e. consider a single (fractional) factorial design with sufficient resolution to estimate the main effects as well as the interactions of interest, including control-control interactions as well as control-noise interactions. In considering a single array, it will often be possible to find a higher resolution design that requires the same number of observations as the Taguchi crossed arrays, or to achieve the same design resolution with less experimental runs. If certain interactions are suspected to exist, this can be considered at the design stage and a design with an appropriate aliasing structure that allows for the estimation of the desired interactions can be found. The fact that Taguchi designs do not handle interactions easily is another major shortcoming. Taguchi designs do allow for interactions *if* it is known which interactions exist *before* the data are collected; for unknown interactions between control factors the Taguchi methodology falls short. The Taguchi method does advocate that follow-up experimentation take place, which seems to be a good procedure but it may somewhat flawed not only due to the inadequacy of the signal to noise ratio but also to due to the poor properties of the original design. (See Lorenzen in Nair, [103], (pages 138-139) where the follow-up design had the same number of runs but higher resolution. In this case the 'best point' was confirmed but an improvement of 30% was also present). Most factorial or fractional factorial designs can be augmented by adding center points and/or axial points. Such designs are commonly used within the context of response surface modeling and experimentation. These and similar designs of this form are the Central Composite Design (CCD), the Box-Behnken three level designs, as well as Plackett-Burnam designs. (Box and Draper) [20], and (Myers, Khuri, and Carter) [97]). Incorporating these ideas within the context of response surface methodology allows for sequential investigation, a feature that, as is often noted, is not generally available with the Taguchi methodology, except in the sense of follow-up confirmation.

It must be remembered that the goal is to find settings that minimize $k(Y-T)^2$ while the tactic is to pick settings that minimize the signal to noise ratio. That the two are equivalent relies directly on the multiplicative error assumption and the further assumption that the parameters can be partitioned into distinct and disjoint subsets, one containing 'adjustment' factors which are used to adjust to the optimal value, one containing 'dispersion' factors which have an effect on the the variation but not the mean, and one containing factors that influence neither the mean nor the variation. However, in an additive error model, where the variance is unrelated to the mean, the minimizations of the signal to noise ratio and the *mse* lead to different 'best' points. That the set of parameters can be partitioned as required is based on the *a priori* assumption that the signal to noise ratio is a function that depends only on some subset of the parameters. The question of when and whether the two are equivalent is covered in (Lèon, Shoemaker, and Kackar) [88]. Furthermore, many different data points representing drastically different means and variances can give rise to the same signal to noise ratio (see Box [21]).

Within the context of a statistical analysis, data transformations are usually performed in order to stabilize the variance of the response. Therefore, in any particular situation, the actual transformation should be stem from a physical or data based understanding of the relation between the mean and the variance, see (Box and Jones) [22]. The reciprocal transformation (or reciprocal squared) may be highly non-linear and is taken independent of the actual data values. The effectiveness of any transformation clearly is related to the actual data; the effect of the reciprocal squared transformation for y between .3 and 2 is very different than the same transformation for y between 20 and 25. The effect of a transformation is well known to be related to the magnitude of the sample quantity, y_{max}/y_{min}. Another criticism of the signal to noise ratio and the issue of data transformation is that both the presence and magnitude of effects are related to the metric chosen by the experimenter. For this reason many people feel that if a transformation is to be done, it should be one suggested by the data, not one chosen beforehand. Lambda plots (Box) [21] are helpful in determining an appropriate transformation, the Taguchi signal to noise ratio is just *one* transformation. It should be noted that this transformation is known to be helpful when σ is proportional to μ (Bartlett) [12].

To summarize, the major complaints against the Taguchi Method are large and expensive designs, the poor ability to allow for interactions, the lack of sequential investigation, the *a priori* assumption of a multiplicative error model, and the inadequacy of the signal to noise ratio. New ideas that fall mostly within the framework of RSM but could apply some of the Taguchi methods include multiple response analysis, sequential design/analysis, the realization that system variability may itself vary within the design region, and non-parametric design (Myers, Khuri, and Carter) [97].

2. GENERAL ALTERNATIVES TO TAGUCHI

Many of those who most strongly voice criticisms of the Taguchi method favor what is known as Response Surface Methodology, or RSM. Response surface methods and methodologies began in 1951, with the work of Box and Wilson (Myers, Khuri, and Carter) [97]. In this review paper, the authors propose one definition for RSM as "*a collection of tools in design or data analysis that enhance the exploration of a region of design variables in one or more responses*". The interest in exploring the response throughout a region is very much different than the Taguchi method of 'picking the best' from what was observed. Applications of RSM in biological sciences, food science, social sciences, physical sciences, engineering and other general industrial situations are also offered in this paper. The underlying premise of RSM is that some response, typically denoted η, is a function of some set of design variables, say $x_1, x_2, ..., x_k$. Although the exact functional relationship between η and $\underset{\sim}{x}$ is generally unknown, the assumption is made that this exact relation can be approximated, at least locally, by a polynomial function of the $x's$. Actual data collected, typically denoted y, is expressed as $y = \eta + \varepsilon$, (Box and Draper) [20]. In most cases the approximating function will be a first or second degree polynomial. The two most common models are thus:

$$\eta = \beta_0 + \beta_1 x_1 + ... + \beta_k x_k \tag{2.1}$$

and

$$\eta = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} {x_i}^2 + \sum_{i<j} \beta_{ij} x_i x_j \tag{2.2}$$

In vector notation these can be written as $\eta = \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta}$ and $\eta = \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x}$, respectively. Here, $\underset{\sim}{x} = (x_1, x_2, ..., x_k)$ is a k-vector of input variables, while β_0, $\underset{\sim}{\beta}$, and $\underset{\sim}{B}$ represent a scalar parameter, a k-dimensional parameter vector, and a k by k symmetric matrix of parameters, respectively. Some assumptions are required on the error associated with the response, assuming that this error follow a $N(0, \sigma^2)$ distribution for some σ^2 allows the researcher to employ many of the tools that accompany classical least squares theory. Inherent to the RSM framework is the idea of sequential investigation. This concept is not a part of the Taguchi methodology other than in follow-up or confirmation of the 'best' design point. Sequential investigation looks for a possible *improvement* in the quality characteristic. This improvement may require settings of factors that were not part of the original experiment. By fitting a model, it becomes possible to *estimate* the response (and possibly the variation) throughout the entire design region, suggesting areas where the response may be closer to target, or other areas where the variation is much less, or is more stable. In contrast to sequential investigation, the Taguchi method looks at optimization, generally considering only design points at which data were actually collected. Remember that the Taguchi inner array is often highly fractionated, which means that many 'potential' design points were *not* included in the inner array. In using response surface methods the researcher conducts a designed experiment, estimates the necessary parameters to fit a model, checks the adequacy of the model (lack of fit test), determines or guesses where improvement will or might take place, and then conducts another experiment with design points concentrated around the area of suspected improvement. This process could be repeated as often as needed but careful planning and experimentation will keep the number of experiments and observations to a minimum. This parallels the idea of trying to understand the process, a major tenet of those in quality circles.

In most response surface situations, all of the 'x' variables in the model can generally be placed at arbitrary levels and are not considered random. To compare directly with the Taguchi methodology, the response surface model needs to be expanded to consider noise variables as well as potential interactions between noise variables and control variables. In many cases it will be relatively easy to observe and record the noise variables. In such situations it may also be possible to place a non-subjective prior distribution on the noise variables. Based on an initial experiment, the quality characteristic could be modeled as a response of *both* the noise variables and the control variables, typically a polynomial of first or second degree. Specifically, if we let Y denote some quality characteristic of interest, we can fit a general model of the form:

$$Y = Y_{xz} = \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} + \underset{\sim}{z}'\gamma + \underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z} + \underset{\sim}{z}'\underset{\sim}{D}\underset{\sim}{x} + \varepsilon \tag{2.3}$$

(Box and Jones) [22]. In this model, $\underset{\sim}{x}$ represents a k-vector of design variables, $\underset{\sim}{z}$ represents a p-dimensional random vector of noise or environmental variables, and ε represents error, usually one assumes $\varepsilon \sim N(0, \sigma^2)$. The parameters β_0, $\underset{\sim}{\beta}$, $\underset{\sim}{B}$, γ, $\underset{\sim}{C}$, $\underset{\sim}{D}$, and σ^2 are generally unknown.

Within the context of sequential investigation, the researcher now would like to know which design points should be considered for the *next* experiment, making use of the current fitted model, realizing that the fitted model is based on parameter estimates, not parameters, and after integrating over the p-dimensional prior on $\underset{\sim}{z}$, the vector of noise variables. Many criterion are available for deciding what makes a new design point (or a new design matrix) optimal. These include D-optimality, A-optimality, minimum bias, minimum variance of prediction, etc. A very common goal is to minimize expected mean square relative to a desired or specified target value. When the concern is for what will happen in the future, the mean square error of prediction becomes a major concern (Allen) [4],(Dwivedi and Srivastava) [41]. Noise factors may be regarded as random regressors, thus changing the interpretation of the regression model slightly, see (Narula) [101], (Reilman, Gunst, and Lakshminarayanan) [115], (Shaffer) [122], (Walls and Weeks) [140], and (Kackar and Harville) [77] for various viewpoints concerning random regressors. In some instances, the response surface may depend on both quantitative and qualitative factors, see (Draper and John) [40]. Various approaches to the dual-response problem are considered in (Castillo and Montgomery) [29], (Vining and Myers) [139] and (Gan) [51].

3. RESPONSE SURFACE ALTERNATIVES

A very common statistical measure of performance is squared error loss, or expected squared error loss. This concept has been used by statisticians for many years but the increased use of Taguchi methods has made many people, particularly engineers and others in industrial situations, realize that *any* deviation from target is detrimental, and that considering only whether or not a part is within specification limits can lead to a false sense of security about a process. Inspection plans concerned only about specification limits without considering variation around a target value can also lead to distributions that are almost uniformly spread across the specification limits, as opposed to being concentrated at the target value. The previously mentioned example of Sony-USA compared to Sony-Japan is a classic example of this phenomenon. (Sullivan, [124]). Within the framework of a Taguchi design the quantity to minimize would be $E(Y-T)^2$, where Y is the characteristic of interest and T represents the target value. Inner and outer arrays would be crossed and signal to noise ratios would be calculated to determine which settings of the design variables would minimize squared error loss. Recall that although the goal is to minimize the mse, the Taguchi criterion is actually some signal to noise ratio.

Here a different formulation will be considered in an effort to improve on standard industry practice. Let Y represent the quality characteristic of interest and recall the general response surface model

$$Y = Y_{xz} = \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} + \underset{\sim}{z}'\underset{\sim}{\gamma} + \underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z} + \underset{\sim}{z}'\underset{\sim}{D}\underset{\sim}{x} + \varepsilon \tag{3.1}$$

(Box and Jones) [22]. In this model, $\underset{\sim}{x}$ represents a k-dimensional vector of design variables, $\underset{\sim}{z}$ represents a p-dimensional random vector of noise variables, and ε represents error, usually it is assumed that $\varepsilon \sim N(0, \sigma^2)$. The parameters β_0, $\underset{\sim}{\beta}$, $\underset{\sim}{B}$, $\underset{\sim}{\gamma}$, $\underset{\sim}{C}$,

$\underset{\sim}{D}$, and σ^2 are generally unknown. This model allows for pure quadratic effects x_i^2 or z_j^2, as well as second order terms such as $x_i x_j$, $x_i z_j$, and $z_i z_j$.

If we consider the noise variables as being part of an environment space, we could first integrate over this environment space and then attempt to minimize the mean squared error. Specifically, the squared error loss would be:

$$\int_{Z_1} \cdots \int_{Z_p} \int_{Y|\underset{\sim}{Z}} (Y - T)^2 \; f_{\underset{\sim}{Z}}(\underset{\sim}{z}) \; f_{Y|\underset{\sim}{Z}}(y|\underset{\sim}{z}) \; dy|\underset{\sim}{z} \; d\underset{\sim}{z} \tag{3.2}$$

Here it assumed that $\underset{\sim}{z} \sim N_p(\underset{\sim}{\mu}_e, \underset{\sim}{A})$ and, independent of $\underset{\sim}{z}, \varepsilon \sim N(0, \sigma^2)$, while all other terms are constants, possibly unknown. It is assumed that the mean, $\underset{\sim}{\mu}_e$, is known and that the covariance matrix, $\underset{\sim}{A}$, is known and is positive definite.

In the most general case, namely

$$\begin{aligned} Y_{xz} &= \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} + \underset{\sim}{z}'\gamma + \underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z} + \underset{\sim}{z}'\underset{\sim}{D}\underset{\sim}{x} + \varepsilon \\ &\equiv B(\underset{\sim}{x}) + \underset{\sim}{z}'\gamma + \underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z} + \underset{\sim}{z}'\underset{\sim}{D}\underset{\sim}{x} + \varepsilon \end{aligned}$$

we have

$$E(Y) = \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} + \underset{\sim}{\mu}_e'(\gamma + \underset{\sim}{D}\underset{\sim}{x}) + \underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{\mu}_e + tr(\underset{\sim}{A}\underset{\sim}{C}) \tag{3.3}$$

$$\begin{aligned} Var(Y) &= \sigma^2 + \gamma'\underset{\sim}{A}\gamma + \underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{D}\underset{\sim}{x} + Var(\underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z}) \\ &+ 2[cov(\underset{\sim}{z}'\gamma, \underset{\sim}{z}'\underset{\sim}{D}\underset{\sim}{x}) + cov(\underset{\sim}{z}'\underset{\sim}{D}\underset{\sim}{x}, \underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z}) + cov(\underset{\sim}{z}'\gamma, \underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z})] \end{aligned} \tag{3.4}$$

where

$$Var(\underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z}) = 2tr(\underset{\sim}{C}\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{A}) + 4\underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{\mu}_e$$

$$cov(\underset{\sim}{z}'\gamma, \underset{\sim}{z}'\underset{\sim}{D}\underset{\sim}{x}) = \underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\gamma, \quad cov(\underset{\sim}{z}'\underset{\sim}{D}\underset{\sim}{x}, \underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z}) = 2\underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{\mu}_e$$

$$cov(\underset{\sim}{z}'\gamma, \underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z}) = 2\gamma'\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{\mu}_e$$

thus

$$Var(Y) = \underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{D}\underset{\sim}{x} + 2\underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\gamma + 4\underset{\sim}{x}'\underset{\sim}{D}\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{\mu}_e + \sigma^2 + Var(\underset{\sim}{z} \; only) \tag{3.5}$$

(See Seber, p41#12, p40 #4, [121]) where σ^2 is the variance in the response and $Var(\underset{\sim}{z} \; only)$ represents variation due to the noise variables but independent of the value of $\underset{\sim}{x}$. These pieces may be ignored when determining the values of $\underset{\sim}{x}$ that minimize the mse. Therefore, (ignoring some terms independent of $\underset{\sim}{x}$)

$$\begin{aligned} E(Y-T)^2 &= \underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{D}\underset{\sim}{x} + 2\underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{\gamma} + 4\underset{\sim}{x}'\underset{\sim}{D}\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{\mu}_e) \\ &\quad + (\beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} + \underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{\mu}_e + \underset{\sim}{\mu}_e'\underset{\sim}{\gamma} + \underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{\mu}_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T)^2 \end{aligned}$$

the first term is $Var(Y)$, the second is the squared bias, $(E(Y)-T)^2$. Considered as function of $\underset{\sim}{x}$, this may be written as

$$\begin{aligned} &\underset{\sim}{x}'[\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{D} + (\underset{\sim}{\beta} + \underset{\sim}{D}'\underset{\sim}{\mu}_e)(\underset{\sim}{\beta} + \underset{\sim}{D}'\underset{\sim}{\mu}_e)' + 2B(\beta_0 + \underset{\sim}{\mu}_e'\underset{\sim}{\gamma} + \underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{\mu}_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T)]\underset{\sim}{x} \\ &\quad + 2\underset{\sim}{x}'[\underset{\sim}{D}'\underset{\sim}{A}(\underset{\sim}{\gamma} + 2\underset{\sim}{C}\underset{\sim}{\mu}_e) + (\underset{\sim}{\beta} + \underset{\sim}{D}'\underset{\sim}{\mu}_e)(\beta_0 + \underset{\sim}{\mu}_e'\underset{\sim}{\gamma} + \underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{\mu}_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T)] \\ &\qquad + (\underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x})^2 + 2\underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x}(\underset{\sim}{x}'(\underset{\sim}{\beta} +' \underset{\sim}{D}'\underset{\sim}{\mu}_e)) \end{aligned}$$

This is fourth degree function of $\underset{\sim}{x}$, but all of the third and fourth order terms will vanish if the model contains no second order terms in $\underset{\sim}{x}$, i.e. when the $B(\underset{\sim}{x})$ term is strictly linear in $\underset{\sim}{x}$, when $B(\underset{\sim}{x})= \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta}$.

3.1 Case 1

In the simplest case the model is given by:

$$y_{xz} = \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} + \underset{\sim}{z}'\underset{\sim}{\gamma} + \varepsilon$$

This model is quadratic in $\underset{\sim}{x}$ and linear or first order in $\underset{\sim}{z}$, with no interaction between noise variables and design variables. For this model, it can be shown that, after integrating over $\underset{\sim}{z}$, Y follows a normal distribution, with mean and variance

$$\beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} + \underset{\sim}{\mu}_e'\underset{\sim}{\gamma}, \qquad \sigma^2 + \underset{\sim}{\gamma}'\underset{\sim}{A}\underset{\sim}{\gamma}$$

In this situation the mean squared error reduces to the following quadratic function of $B(\underset{\sim}{x})$:

$$\begin{aligned} E(Y-T)^2 &= B(\underset{\sim}{x})^2 + 2B(\underset{\sim}{x})(\underset{\sim}{\mu}_e'\underset{\sim}{\gamma} - T) + \sigma^2 + (\underset{\sim}{\gamma}'\underset{\sim}{A}\underset{\sim}{\gamma}) + (\underset{\sim}{\mu}_e'\underset{\sim}{\gamma} - T)^2 \\ &= (B(\underset{\sim}{x}) + \underset{\sim}{\mu}_e'\underset{\sim}{\gamma} - T)^2 + \sigma^2 + (\underset{\sim}{\gamma}'\underset{\sim}{A}\underset{\sim}{\gamma}) \end{aligned}$$

This quadratic is minimized at $B(\underset{\sim}{x}) = T - \underset{\sim}{\mu}'_e\gamma$, which is the same as $E(Y) = T$. (Note that the previous derivations explicitly assume that all necessary parameters are known. In practice this will rarely if ever occur. The implications of using parameter estimates are discussed in the next chapter.) The squared error loss at $B(\underset{\sim}{x}) = T - \underset{\sim}{\mu}'_e$ is $\sigma^2 + \gamma'\underset{\sim}{A}\gamma$. Notice that this is simply the overall variance of Y, which is equivalent to the mean squared error when the design points are such that $E(Y) = T$, i.e. when an unbiasedness condition is satisfied. For this model, the variance of Y does not involve $\underset{\sim}{x}$, and thus the minimum mse occurs when new design points satisfy $E(Y) = T$. Specifically, this means that new design points should satisfy either

$$\begin{aligned} &a) \qquad \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} = T - \underset{\sim}{\mu}'_e\gamma \\ or \quad &b) \; \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} = T - \underset{\sim}{\mu}'_e\gamma \end{aligned}$$

Knowing the marginal distribution of y in this situation allows for confidence intervals to be produced; prediction intervals are more complicated since any future value of Y will also involve a random value $\underset{\sim}{z}$.

3.2 Case 2

In this case the model is given by:

$$y_{xz} = \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} + \underset{\sim}{z}'\gamma + \underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z} + \varepsilon,$$

This allows for pure quadratic terms and interactions within both the design region and the noise region but does not allow for interactions across the two regions. For this model the mse is

$$\begin{aligned} & B(\underset{\sim}{x})^2 + 2B(\underset{\sim}{x})[\underset{\sim}{\mu}'_e\gamma + \underset{\sim}{\mu}'_e\underset{\sim}{C}\underset{\sim}{\mu}_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T] \\ + \;\; & \sigma^2 + \gamma'\underset{\sim}{A}\gamma + (\underset{\sim}{\mu}'_e\gamma - T)^2 + \; E_z[T - \underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z}]^2 + 2E_z[\underset{\sim}{z}'\gamma\underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z}] - T^2 \end{aligned}$$

As in case 1, $Var(Y)$ does not involve $\underset{\sim}{x}$, so the mse is again minimized by requiring new design points to be unbiased. The mse is again a quadratic function of $B(\underset{\sim}{x})$, and is minimized at

$$B(\underset{\sim}{x}) \;=\; T - \underset{\sim}{\mu}'_e\gamma - \underset{\sim}{\mu}'_e\underset{\sim}{C}\underset{\sim}{\mu}_e - tr(\underset{\sim}{A}\underset{\sim}{C}),$$

which means we must look for design points satisfying

$$a)\ \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} = T - \underset{\sim}{\mu}_e'\underset{\sim}{\gamma} - \underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{\mu}_e - tr(\underset{\sim}{A}\underset{\sim}{C})$$

$$or\ b)\ \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} = T - \underset{\sim}{\mu}_e'\underset{\sim}{\gamma} - \underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{\mu}_e - tr(\underset{\sim}{A}\underset{\sim}{C})$$

For this model, it is much more complicated to integrate over the density of $\underset{\sim}{z}$, since the conditional density of Y now contains terms involving up to the fourth power of the z_i. It is easy to show, however, that, in this case, using (3.4) and (3.5),

$$E(Y) = \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} + \underset{\sim}{\mu}_e'\underset{\sim}{\gamma} + \underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{\mu}_e + tr(\underset{\sim}{A}\underset{\sim}{C}),$$

$$Var(Y) = \sigma^2 + \underset{\sim}{\gamma}'\underset{\sim}{A}\underset{\sim}{\gamma} + 2tr(\underset{\sim}{C}\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{A}) + 4\underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{\mu}_e + 4\underset{\sim}{\gamma}'\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{\mu}_e$$

3.3 Case 3

As the models presented have allowed for random effects to influence the response, it seems reasonable, or even probable, that this influence may depend on the levels of certain control variables. The Taguchi method implicitly assumes that the variance of the quality characteristic is not equal at all control settings given in the inner array. This essentially implies that the design space and the environment space interact. The simplest model to handle this situation is given by:

$$\begin{aligned} y_{xz} &= \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} + \underset{\sim}{z}'\underset{\sim}{\gamma} + \underset{\sim}{z}'\underset{\sim}{D}\underset{\sim}{x} + \varepsilon, \\ &= B(\underset{\sim}{x}) + \underset{\sim}{z}'\underset{\sim}{\gamma} + \underset{\sim}{z}'\underset{\sim}{D}\underset{\sim}{x} + \varepsilon \\ &= B(\underset{\sim}{x}) + \underset{\sim}{z}'(\underset{\sim}{\gamma} + \underset{\sim}{D}\underset{\sim}{x}) + \varepsilon \end{aligned}$$

This represents a model that is linear in $\underset{\sim}{z}$, quadratic in $\underset{\sim}{x}$ and allows for interaction between design and noise variables. As far as the random variable $\underset{\sim}{z}$ is concerned, this is equivalent to model one, with the substitution $\underset{\sim}{\gamma}$ becoming $\underset{\sim}{\gamma} + \underset{\sim}{D}\underset{\sim}{x}$. Since this substitution involves $\underset{\sim}{x}$, the choice of optimal new design points will not, however, be the same as in model one. Furthermore, $Var(Y)$ now does depend on $\underset{\sim}{x}$ and thus being unbiased may not give the minimum mse. This model has mse

$$\begin{aligned} B(\underset{\sim}{x})^2 + 2B(\underset{\sim}{x})[\underset{\sim}{\mu}_e'(\underset{\sim}{\gamma} + \underset{\sim}{D}\underset{\sim}{x}) - T] + (\underset{\sim}{\gamma} + \underset{\sim}{D}\underset{\sim}{x})'\underset{\sim}{A}(\underset{\sim}{\gamma} + \underset{\sim}{D}\underset{\sim}{x}) \\ + \ (\underset{\sim}{\mu}_e'(\underset{\sim}{\gamma} + \underset{\sim}{D}\underset{\sim}{x}) - T)^2 + \sigma^2 \end{aligned}$$

Since the difference between this model and model one involves only $\underset{\sim}{x}$, we can again calculate the density of Y, after integrating over $\underset{\sim}{z}$, as being normal, with

$$E(Y) = \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} + \underset{\sim}{\mu}_e'(\gamma + \underset{\sim}{D}\underset{\sim}{x}), \quad Var(Y) = \sigma^2 + (\gamma + \underset{\sim}{D}\underset{\sim}{x})'\underset{\sim}{A}(\gamma + \underset{\sim}{D}\underset{\sim}{x})$$

Notice that the mse is no longer a quadratic function of $B(\underset{\sim}{x})$ as it now also involves quadratic terms in both $B(\underset{\sim}{x})$ and $\underset{\sim}{D}\underset{\sim}{x}$, as well as the higher order terms stemming from the product of $B(\underset{\sim}{x})$ and $\underset{\sim}{D}\underset{\sim}{x}$. For this model, the variance of Y is now a quadratic function of $\underset{\sim}{x}$ and is minimized at $\underset{\sim}{x} = -(\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{D})^{-1}\underset{\sim}{D}'\underset{\sim}{A}\gamma$. Satisfying the minimum variance condition may place the mean response well away from the target value or require values of $\underset{\sim}{x}$ out of the range of the design space.

3.3.1 Case 3, Second Order Model

If the model does allow for (or require) second order terms in $\underset{\sim}{x}$, i.e. $B(\underset{\sim}{x}) = \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x}$, then the mean square will contain third and fourth order terms due the $B(\underset{\sim}{x}) * \underset{\sim}{D}\underset{\sim}{x}$ term and the $B(\underset{\sim}{x})^2$ term. Specifically, we have

$$\begin{aligned} E(Y-T)^2 &= \underset{\sim}{x}'[\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{D} + \underset{\sim}{\beta}\underset{\sim}{\beta}' + 2\underset{\sim}{\beta}\underset{\sim}{\mu}_e'\underset{\sim}{D} + \underset{\sim}{D}'\underset{\sim}{\mu}_e\underset{\sim}{\mu}_e'\underset{\sim}{D} + 2\underset{\sim}{B}(\beta_0 + \underset{\sim}{\mu}_e'\gamma - T)]\underset{\sim}{x} \\ &+ 2\underset{\sim}{x}'[\underset{\sim}{D}'\underset{\sim}{A}\gamma + (\underset{\sim}{\beta} + \underset{\sim}{D}'\underset{\sim}{\mu}_e)(\beta_0 + \underset{\sim}{\mu}_e'\gamma - T)] \\ &+ (\underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x})^2 + 2\underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x}(\underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{\mu}_e) \end{aligned}$$

Obviously the higher order terms involving $\underset{\sim}{x}$ make it more difficult to minimize the mse and stay within the design or feasibility region.

3.3.2 Case 3, First Order Model

If the term $B(\underset{\sim}{x})$ is given by $B(\underset{\sim}{x}) = \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta}$, then the mse is again a quadratic function of $\underset{\sim}{x} = (x_1, x_2, , \ldots, x_k)$, although not the same function as in case 1 or case 2. Under the assumption that $\underset{\sim}{B} = \underset{\sim}{0}$, the mean squared error is

$$\begin{aligned} &\underset{\sim}{x}'[\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{D} + \underset{\sim}{\beta}\underset{\sim}{\beta}' + 2\underset{\sim}{\beta}\underset{\sim}{\mu}_e'\underset{\sim}{D} + \underset{\sim}{D}'\underset{\sim}{\mu}_e\underset{\sim}{\mu}_e'\underset{\sim}{D}]\underset{\sim}{x} \\ &+ 2\underset{\sim}{x}'[\underset{\sim}{D}'\underset{\sim}{A}\gamma + (\underset{\sim}{\beta} + \underset{\sim}{D}'\underset{\sim}{\mu}_e)(\beta_0 + \underset{\sim}{\mu}_e'\gamma - T)] \\ &+ (\beta_0 + \underset{\sim}{\mu}_e'\gamma - T)^2 + \sigma^2 \end{aligned}$$

Notice the above function is convex in $\underset{\sim}{x}$, thus a unique minimum occurs but such a point may not be in the design region.

3.4 Case 4

Depending on the situation, it may be necessary to include second order terms in the noise variables in order to more accurately model the response. Generally a model that includes these second order terms in the noise variables would also contain terms up to second degree in the control variables, as well as possible interactions between the noise and control variables. A model that allows for all of this is given by:

$$y_{xz} = \beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} + \underset{\sim}{z}'\gamma + \underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z} + \underset{\sim}{z}'\underset{\sim}{D}\underset{\sim}{x} + \varepsilon$$

The *mse* is now given by:

$$B(\underset{\sim}{x})^2 + 2B(\underset{\sim}{x})[\mu_e(\gamma + \underset{\sim}{D}\underset{\sim}{x}) + \mu_e'\underset{\sim}{C}\mu_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T] + [\mu_e(\gamma + \underset{\sim}{D}\underset{\sim}{x}) - T]^2$$
$$+[(\gamma + \underset{\sim}{D}\underset{\sim}{x})'\underset{\sim}{A}(\gamma + \underset{\sim}{D}\underset{\sim}{x})] + 2E[\underset{\sim}{z}'(\gamma + \underset{\sim}{D}\underset{\sim}{x})(\underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z})] + \sigma^2 + E[T - \underset{\sim}{z}'\underset{\sim}{C}\underset{\sim}{z}]^2 - T^2$$

This can be simplified to (again, ignoring terms independent of $\underset{\sim}{x}$)

$$(\underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x})^2 + 2\underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x}(\mu_e'\gamma + \mu_e'\underset{\sim}{C}\mu_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T)$$
$$+ 2\underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x}(\underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{D}'\mu_e)$$
$$+ \underset{\sim}{x}'\underset{\sim}{D}'\mu_e\mu_e'\underset{\sim}{D}\underset{\sim}{x} + \underset{\sim}{x}\underset{\sim}{\beta}\underset{\sim}{\beta}'\underset{\sim}{x} + \underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{D}\underset{\sim}{x} + 2\underset{\sim}{x}'\underset{\sim}{\beta}\mu_e'\underset{\sim}{D}\underset{\sim}{x}$$
$$+ 2\underset{\sim}{x}'\underset{\sim}{\beta}(\mu_e'\gamma + \mu_e'\underset{\sim}{C}\mu_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T) + 2\underset{\sim}{x}'\underset{\sim}{D}'\mu_e(\mu_e'\gamma + \mu_e'\underset{\sim}{C}\mu_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T)$$
$$+ 2\underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\gamma + 4\underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{C}\mu_e$$

All of the above may be factored and grouped as

$$\underset{\sim}{x}'[\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{D} + \underset{\sim}{\beta}\underset{\sim}{\beta}' + 2\underset{\sim}{\beta}\mu_e'\underset{\sim}{D} + \underset{\sim}{D}'\mu_e\mu_e'\underset{\sim}{D} + 2\underset{\sim}{B}(\beta_0 + \mu_e'\gamma + \mu_e'\underset{\sim}{C}\mu_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T)]\underset{\sim}{x}$$
$$+ 2\underset{\sim}{x}'[\underset{\sim}{D}'\underset{\sim}{A}(\gamma + 2\underset{\sim}{C}\mu_e) + (\underset{\sim}{\beta} + \underset{\sim}{D}'\mu_e)(\beta_0 + \mu_e'\gamma + \mu_e'\underset{\sim}{C}\mu_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T)]$$
$$+ (\underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x})^2 + 2\underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x}(\underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{D}'\mu_e)$$

3.4.1 Case 4, Second Order Model

When the response is quadratic in $\underset{\sim}{x}$, the mse is fourth degree in $\underset{\sim}{x}$. It may prove difficult to minimize the mse, due to the higher order terms in $\underset{\sim}{x}$. A slightly different approach would be to require that our new design points are unbiased, and then minimize the variance of Y that depends on $\underset{\sim}{x}$, namely we want

$$min\{\underset{\sim}{x}\} \quad \underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{D}\underset{\sim}{x} + 2\underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\gamma + 4\underset{\sim}{x}'\underset{\sim}{D}\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{\mu}_e$$

subject to:

$$\beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} + \underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{\mu}_e = T - \underset{\sim}{\mu}_e'\gamma - \underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{\mu}_e - tr(\underset{\sim}{A}\underset{\sim}{C})$$

We also have the adder restriction that the the point must be in the design region. In general, minimizing the variance while requiring unbiasedness means we must minimize a second order function of $\underset{\sim}{x}$ subject to a second order condition on $\underset{\sim}{x}$. Depending on the circumstance, it may happen that the bias relative to target is more important than the variance. One method to handle the relative importance between the variance and the squared bias is to minimize the function

$$g_\lambda(\underset{\sim}{x}) = \lambda * Var(Y) + (1-\lambda) * bias^2, \quad 0 \ < \ \lambda \ < \ 1$$

for various values of λ, with $\lambda = .5$ being equivalent to minimizing mse. For more details on this and how to choose λ, see (Box and Jones) [22].

3.4.2 Case 4, First Order Model

If the model is linear in $\underset{\sim}{x}$, meaning that the $B(\underset{\sim}{x})$ term is $\beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta}$, then the two conditions are for the constrained optimization problem of minimizing the variance subject to the unbiasedness condition (ignoring the constraint of being within the design space) are equivalent to

$$min\{\underset{\sim}{x}\} \quad \underset{\sim}{x}'\underset{\sim}{H}\underset{\sim}{x} + \underset{\sim}{x}'\underset{\sim}{c} \ \ such\ that\ \underset{\sim}{x}'\underset{\sim}{d} = k$$

Here, $\underset{\sim}{H} = \underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{D}$ and $\underset{\sim}{c} = 2\underset{\sim}{D}'\underset{\sim}{A}\gamma + 4\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{\mu}_e$. Thus the minimum variance unbiased condition takes the form of a somewhat standard quadratic programming problem, and can be solved fairly easily (see [118]) if the matrix $\underset{\sim}{H}$, is positive semidefinite, as it generally will be; however the programming problem is solved under the added condition that $\underset{\sim}{x} > \underset{\sim}{0}$, which presents a second condition which may be impossible to meet. A further simplification under the assumption that $\underset{\sim}{B} = \underset{\sim}{0}$ is that the entire mse simplifies to (ignoring terms independent of $\underset{\sim}{x}$)

$$\underset{\sim}{x}'[\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{D} + (\underset{\sim}{\beta} + \underset{\sim}{D}'\underset{\sim}{\mu}_e)(\underset{\sim}{\beta} + \underset{\sim}{D}'\underset{\sim}{\mu}_e)' + 2\underset{\sim}{\beta}(\beta_0 + \underset{\sim}{\mu}_e'\underset{\sim}{\gamma} + \underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{\mu}_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T)]x$$
$$+ \;\; 2\underset{\sim}{x}'[\underset{\sim}{D}'\underset{\sim}{A}(\underset{\sim}{\gamma} + 2\underset{\sim}{C}\underset{\sim}{\mu}_e) + (\beta + \underset{\sim}{D}'\underset{\sim}{\mu}_e)(\beta_0 + \underset{\sim}{\mu}_e'\underset{\sim}{\gamma} + \underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{\mu}_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T)]$$

Notice that this is now only second order in $\underset{\sim}{x}$ and may be minimized much more easily, (as compared to the previous model), namely

$$\underset{\sim}{x}^* = -[\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{D} + (\underset{\sim}{\beta} + \underset{\sim}{D}'\underset{\sim}{\mu}_e)(\underset{\sim}{\beta} + \underset{\sim}{D}'\underset{\sim}{\mu}_e)' + 2\underset{\sim}{B}(\beta_0 + \underset{\sim}{\mu}_e'\underset{\sim}{\gamma} + \underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{\mu}_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T)]^{-1}$$
$$[\underset{\sim}{D}'\underset{\sim}{A}(\underset{\sim}{\gamma} + 2\underset{\sim}{C}\underset{\sim}{\mu}_e) + (\beta + \underset{\sim}{D}'\underset{\sim}{\mu}_e)(\beta_0 + \underset{\sim}{\mu}_e'\underset{\sim}{\gamma} + \underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{\mu}_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T)]$$

Here, $\underset{\sim}{x}^*$ is the point that minimizes the mse. As the model gets more complicated, the corresponding mse also becomes more complicated, and will involve higher powers of $\underset{\sim}{x}$, higher moments of $\underset{\sim}{z}$ and the corresponding cross-products. It can be shown, however, that, although the marginal density is not normal, one still has, using (3.4) and (3.5),

$$E(Y) = B(\underset{\sim}{x}) + \underset{\sim}{\mu}_e'(\underset{\sim}{\gamma} + \underset{\sim}{D}\underset{\sim}{x}) + \underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{\mu}_e + tr(\underset{\sim}{A}\underset{\sim}{C})$$

$$Var(Y) = \sigma^2 + (\gamma + \underset{\sim}{D}\underset{\sim}{x})'\underset{\sim}{A}(\gamma + \underset{\sim}{D}\underset{\sim}{x}) + 2tr(\underset{\sim}{C}\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{A}) + 4\underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{\mu}_e + 4(\gamma + \underset{\sim}{D}\underset{\sim}{x})'\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{\mu}_e$$

4. NEW DESIGN POINTS - EFFECT OF PARAMETER ESTIMATION

For each case given in chapter three, the solution determined by $E(Y) = T$ is actually a surface, either of first or second degree in $\underset{\sim}{x} = (x_1, x_2, \ldots x_k)'$; minimizing the mse is equivalent to finding the level curves of a function that may be up fourth order in $\underset{\sim}{x}$. However, the development in the previous chapter is based on the assumption that all of the necessary parameters are known, an assumption that will rarely, if ever, be met in practice. Since the goal is to select new design points, the mse of prediction is a critical issue. The variance in prediction stems from three sources: the variance in the response, the variance associated with the noise variables, and the variance induced by making predictions based on parameter estimates. While we hope to minimize the mse of some future observation, we can only do this conditionally, conditional on the parameter estimates we have at the current time. Thus while we would like to minimize (the true mse, dropping some terms independent of $\underset{\sim}{x}$)

$$\begin{aligned} E[(Y-T)^2] &= \underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{D}\underset{\sim}{x} + 2\underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{\gamma} + 4\underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{A}\underset{\sim}{C}\underset{\sim}{\mu}_e \\ &+ (\beta_0 + \underset{\sim}{x}'\underset{\sim}{\beta} + \underset{\sim}{x}'\underset{\sim}{B}\underset{\sim}{x} + \underset{\sim}{x}'\underset{\sim}{D}'\underset{\sim}{\mu}_e + \underset{\sim}{\mu}_e'\underset{\sim}{\gamma} + \underset{\sim}{\mu}_e'\underset{\sim}{C}\underset{\sim}{\mu}_e + tr(\underset{\sim}{A}\underset{\sim}{C}) - T)^2, \end{aligned}$$

we will have to consider an estimate of the true mse, which, (again ignoring some terms independent of $\underset{\sim}{x}$) is given by:

$$\widehat{MSE} = \underset{\sim}{x}'\hat{\underset{\sim}{D}}'\underset{\sim}{A}\hat{\underset{\sim}{D}}\underset{\sim}{x} + 2\underset{\sim}{x}'\hat{\underset{\sim}{D}}'\underset{\sim}{A}\hat{\underset{\sim}{\gamma}} + 4\underset{\sim}{x}'\hat{\underset{\sim}{D}}'\underset{\sim}{A}\hat{\underset{\sim}{C}}\underset{\sim}{\mu}_e \quad (4.1)$$

$$+ (\hat{\beta}_0 + \underset{\sim}{x}'\hat{\underset{\sim}{\beta}} + \underset{\sim}{x}'\hat{\underset{\sim}{D}}'\underset{\sim}{\mu}_e + \underset{\sim}{x}'\hat{\underset{\sim}{B}}\underset{\sim}{x} + \underset{\sim}{\mu}_e'\hat{\underset{\sim}{\gamma}} + \underset{\sim}{\mu}_e'\hat{\underset{\sim}{C}}\underset{\sim}{\mu}_e + tr(\underset{\sim}{A}\hat{\underset{\sim}{C}}) - T)^2 \quad (4.2)$$

The first term represents the variance associated with the noise-control factor interactions, the second term is the squared bias relative to the target value. The estimates could be based on classical least squares theory, but this is not required.