ON THE SENSITIVITY OF DESIRABILITY FUNCTIONS FOR MULTIRESPONSE OPTIMIZATION

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ABSTRACT

Desirability functions have been one of the most important multiresponse optimization technique since the early eighties. Main reasons for this popularity might be counted as the convenience of the implementation of the method and the availability of it in many experimental design software packages. Technique itself involves somehow subjective parameters such as the importance coefficients between response characteristics that are used to calculate overall desirability, weights used in determining the shape of each individual response and the size of the specification band of the response. However, the impact of these sensitive parameters on the solution set is mostly uninvestigated. This paper proposes a procedure to analyze the sensitivity of the important characteristic parameters of desirability functions and their impact on pareto-optimal solution set. The proposed procedure uses the experimental design tools on the solution space and estimates a prediction equation on the overall desirability to identify the sensitive parameters. For illustration, a classical desirability example is selected from the literature and results are given along with the discussion.

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1. Introduction

A typical product or process development problem involves determining the desired values of multiple responses of interest by finding the optimum settings of input variables in a defined solution space. These responses might be the quality characteristics of a product or observed outputs of a manufacturing process. In either case, practitioners face an obvious dilemma of simultaneous optimization of all these response variables. In rare cases, responses of interest do not compete with each other and the problem at hand can be solved by deducting it into a univariate problem. But most of the time an improvement in the desired value of one response variable can only be achieved by the setback in the value(s) of one or more responses. The solution of this dilemma has become one of the most interesting fields of various engineering disciplines since the early seventies under the title of “multiresponse optimization problem”.

By the evolution of Response Surface Methodology (RSM), many optimization schemes have been used to solve the Multiresponse Optimization (MO) problem. Some of these approaches are modelled by optimizing one response subject to other responses set at certain bound values as constraints. Hartmann and Beaumont (1968) involve linear form of this kind of approach where Myers and Montgomery (1995) formulated the problem in a nonlinear manner. Khuri and Conlon (1981) introduced a distance approach, based on the overall closeness of the response variables to their optimal values. Quadratic loss functions of Taguchi (1979) also proved to be effective by many authors such as Pignatiello (1995) and Spiring (1998), in MO.

Desirability functions, originally introduced by Harrington (1965), found extensive use in multiresponse problems in the form proposed by Derringer and Suich (1980).

Applications from the recent literature can be found on various areas including semiconductor scheduling by Dabbas *et al.* (2003), on the optical performance of the broadband tap coupler by Hsu *et al.* (2004) and on the optimization of micellar liquid chromatography by Safa and Hadjmohammadi (2005). Later on, Del Castillo *et al.* (1996) modified these functions in order to make them differentiable in the whole defined space so that modern optimization techniques such as gradient based methods can be applied to solve the problem more efficiently. Today, many popular statistical software packages such as Design-Expert® use desirability functions in their response surface optimization modules.

On the other hand, none of these studies or solver packages focuses on the sensitivity analysis of the optimum results generated. Such an analysis is especially important when using the desirability functions as the preferred method for MO since these functions consist of somehow subjective parameters more than any other optimization method. Thus this paper proposes a sensitivity algorithm to fill this gap in the desirability literature, which can be directly incorporated to the desirability functions methodology without manipulating the solution procedure. Furthermore, utilization of the very same experimental design methods that we use in RSM creates a sequential optimization as well as a flexible sensitivity method and eliminates the implementation of a nonparametric methodology.

The paper is organised as five sections in total. In section 2, desirability function methodology and its use in MO problems is introduced. Later on, a discussion on the marginal rates of substitution between rival responses is given. Section 4 proposes a sensitivity analysis procedure on the parameter set of multiresponse problems solved by desirability functions. Finally, strength and weakness of the proposed procedure is supported along with conclusions and discussions on the results of a popular example from MO literature.

2. Desirability Functions

In a MO problem, simultaneous optimization of all responses is possible by combining them into a single objective function, which basically represents the relationship of all responses that are to be optimized. Only by doing so, one can achieve the ideal balance among the desired response levels. The use of experimental design tools is common to all MO methods to gather the mathematical relationship between independent input variables and resulting responses. This relation can be shown by

$$Y_i = f_i(x_1, x_2, \ldots, x_j) + \varepsilon_i \qquad (1)$$

RSM utilizes the experimental design methods to model this relationship in a functional form and then solves this model in a specified region to find the optimal response values and corresponding input variable levels. Although the form of this relationship is not known in most MO problems, preferably a linear model or a high order polynomial model is tried to be gathered to approximate this relationship. When the order of the model(s) or the number of responses to be optimized is large, desirability functions is a favourable method by means of computational efficiency since RSM is a sequential procedure.

MO via desirability functions comprises the following steps. First an adequate function transforms each determined response level into a desirability score within 0 -1 scale. Then all individual desirability scores are combined on a single overall desirability function, which is optimized to find the optimum set of input variables. This combined mathematical relationship of responses is given as

$$\max\ D = \left(d_1(Y_1)^{k_1} \times d_2(Y_2)^{k_2} \times \ldots \times d_n(Y_n)^{k_n}\right)^{1/\sum_i k_i} \tag{2}$$

where Y_i is the determined level of the response *i*, $d_i(Y_i)$ is the converted desirability score of the associated response and k_i being the relative importance of that response compared to others. Maximization of *overall desirability* function, *D*, will also yield to a value between 0 and 1 in which being close to 1 as much as possible is desired. Individual desirability scores can be determined for any three kinds of questions faced in the multiresponse problems.

Transformation of the response levels into desirability scores can be achieved by using several functions. While founding paper of desirability functions by Harrington proposes exponential functions, in practice, weighted linear functions proposed by Derringer and Suich are far more popular. Weighted linear transformations are flexible in determining the risk associated with deviations from desired response levels. Following are the transformations proposed by these authors:

If the response of interest is a nominal or nominal (target) the best kind of problem, then the proposed individual desirability function is

$$d_i(Y_i) = \begin{cases} 0 & Y_i < LSL \\ \left(\dfrac{Y_i - LSL}{T - LSL}\right)^s & LSL \le Y_i \le T \\ \left(\dfrac{Y_i - USL}{T - USL}\right)^t & T \le Y_i \le USL \\ 0 & Y_i > USL \end{cases} \tag{3}$$

where *LSL* and *USL* are the lower and upper specification limits and *T* is the target value of the associated response Y_i. The weight exponents *s* and *t* specifies the underlying form of the response within the range of interest and how strictly the target is desired.

Similarly, when the response of interest is minimization, then a smaller the better type of desirability function is used as

$$d_i(Y_i) = \begin{cases} 1.0 & Y_i \leq LSL \\ \left(\dfrac{Y_i - USL}{LSL - USL}\right)^s & LSL < Y_i \leq USL \\ 0 & Y_i > USL \end{cases} \tag{4}$$

where *LSL* automatically becomes the desired minimum value. It is the practical lower bound which any value below this would not improve the response.

And when the response of interest is maximization, then a larger the better type of desirability function is used.

$$d_i(Y_i) = \begin{cases} 0 & Y_i < LSL \\ \left(\dfrac{Y_i - LSL}{USL - LSL}\right)^s & LSL \leq Y_i \leq USL \\ 1.0 & Y_i > USL \end{cases} \tag{5}$$

where *USL* automatically becomes the desired maximum value. It is the practical upper bound which any value above this would not improve the response.

Figure 1. Nominal the best desirability function

Figure 2. Smaller the better desirability function

Figure 3. Larger the better desirability function

While the target is best kind of desirability function represents a two-sided transformation, smaller the better and larger the better type of desirability functions are one sided transformations. This can clearly be observed from the shape of each individual desirability function for various settings of their corresponding parameters. For example; in target is best case, for user specified values $s = t = 1$ the desirability function increases linearly towards *T* (target), for $s < 1$, $t < 1$ the function is convex, and for $s > 1$, $t > 1$ the function is concave. Note that weights *s* and *t* provide greater flexibility in assigning the individual desirability within the range of interest. While these weight coefficients denote the desired trend of the response within itself, importance coefficient of each response, *k*'s, associates the priority sequence of all responses so that a comparison between them is possible. Also, the strength of the convexity and concavity form of the responses depend on the size of specification band. Range of the response, defined as the measure between upper and lower specification limit, plays an important role on the individual desirability since *d* decreases as the response *Y* moves away from its target.

3. Trade-off Structure within the Response Surface

The basic necessity of a classic multiresponse (or any multiple objective) problem is to identify the models behaviour under a set of different feasible solutions, which is defined as the pareto-optimal solution domain. This analysis of sensitivity is performed by measuring the robustness of pareto-optimal solution with respect to the trade-offs occurring in the optimal values of the model's response variables. The degree of rivalry between the responses also determines the level of difficulty of finding a compromising solution to the problem at hand.

Trade-off structure within the response surface can be best characterized by the marginal rates of substitution concept. Use of the marginal rates of substitution is first introduced by Keeney and Raiffa (1993) where the rate is calculated by the amount of loss in one response in order to gain a unit from the other. The marginal rate of substitution, λ, of two response variables such as y_1 and y_2, performing in a solution domain with n responses can be calculated from the following

$$\lambda_{y_1,y_2} = \frac{\partial u_{y_1}(y_1, y_2, \ldots, y_n)}{\partial u_{y_2}(y_1, y_2, \ldots, y_n)} \tag{6}$$

This rate may also be obtained graphically by observing the slope of the vector generated with the change in value of y_1 with respect to the improvement in y_2 by a margin of one unit. Kros and Mastrangelo (2001) utilize the marginal rates of substitution concept for the application of desirability functions. Since desirability function combines all objectives in a single maximization form, the marginal rate of substitution between two responses can simply be determined by the ratio of relative importance's, $k_i > 0$ of the responses being investigated as

$$\lambda_{y_1,y_2} = \frac{\partial u_{y_1}(y_1, y_2, \ldots, y_n)}{\partial u_{y_2}(y_1, y_2, \ldots, y_n)} = \frac{k_1}{\sum k_i} \Big/ \frac{k_2}{\sum k_i} = \frac{k_1}{k_2} \tag{7}$$

When no response is dominant to another within response surface ($k_1 = k_2 = \ldots = k_n$), then λ should be equal to one. In all other cases, (7) would determine the trade-off magnitude. For example, the manufacturing of printed circuit boards may involve multiple responses of interest to be optimized such as the maximization of peel bond strength, minimization of catalyser amount, setting the board thickness at a nominal value etc. If the relative importance of the peel bond strength (y_1) is set twice as large (k_1) as the relative importance (k_2) of board thickness (y_2) then the marginal rate of substitution λ_{y_1,y_2} would be equal to two.

However, k_i 's are not the only distinct parameters of desirability functions. Weight coefficients s_i 's and t_i 's and range of the underlying response variable also influences the optimal trade-off frontier and the resulting overall desirability strongly. Influence of these parameters as a whole to the overall desirability and resulting optimal frontier has not found much interest in the literature.

4. Sensitivity Analysis

There exists no customary selection (or determination) procedure for the parameters of desirability functions. The term "*user specified*" is used when these parameters are mentioned in the solution process, which in turn may lead to somehow biased or arbitrary selections. The question that has to be investigated is how sensitive the weight, importance and range parameters are to the desired value of the response. From the managerial point of view, it is likely to decide on cost sensitive values. But as a design or quality engineer this decision has to have statistical basis so that optimization results could be further analyzed. This analysis should check the robustness of the overall desirability to changes in these parameters.

Regardless of the chosen optimization technique, initial approach for a MO problem is archetypal. First we design and conduct the experiments by fitting the observed responses on the certain levels of input variables, generally x_i . By doing so, we try to estimate the linear, quadratic or cubic prediction equation that is most significant for each response. Then the solution efforts try to optimize the levels of input variables which simultaneously produce the most desirable predicted responses within the range of interest. However, the desired values of the responses are only pareto-optimal since these values are subject to change for various settings of the parameters of desirability solution procedure. The strength of pareto-optimality should be investigated with respect to these parameters in order to seek alternative cost effective solutions.

The general approach can be extended to include a sensitivity analysis by varying the parameters to certain upper and lower edges and analyze the effect of this on overall desirability by obtaining a prediction equation in which the overall desirability itself becomes the response of interest. The procedure includes following steps.

1. Assign the upper and lower edges for each parameter that has symmetric distances from the origin such as one half for the lower edge and twice as large for upper edge. For example; importance parameter, which is usually set to one or equal in every response should be selected as the half of original value for lower edge, and should be selected twice as large for its upper edge. If the origin (centre point) is selected as two, then lower edge should be one and upper edge should be four. Assignment of edges for weight parameters, s and t, will be done in a similar fashion. For range parameter, edges may also be selected by narrowing to half of the original range for lower and widening by one half for upper edge.
2. Actual settings then must be coded for the necessary factorial design. This design may or may not include the centre points. However inclusion of these points is useful for identifying the effects of interactions between parameters. Note that for any response Y,

three factors should be included to design. As the number of responses increase, the number of runs necessary to complete a full factorial design rapidly increases.

4. Solve the multiresponse problem for each run and obtain the overall desirability value that will be used as the response value in the corresponding sensitivity design.

5. Find the most significant model, model terms, and associated prediction equation on the overall desirability.

6. Coefficients and signs of the factors in this prediction equation should identify the sensitivity of each parameter. While negative valued factors will decrease the overall desirability, positive values will improve it. Regardless of the sign, coefficients close to zero could be marked as insensitive.

Note that this procedure is a sequential procedure and requires the desirability function solution gathered from the settings given in each run. Each of these runs includes the separate use of importance, weight, and range parameters in optimum response values as design variables. For this reason selection of design plays an important role. If the number of responses is two then a design such as Box-Behnken can be selected to include centre points. However, when the number of responses is more than two, then use of fractional factorial designs should be considered to gather a significant model with a small set of design points.

5. Example

The chemical reaction experiment of Myers and Montgomery (1995) is a popular example widely used in the desirability literature (originally presented in Box, Hunter, and Hunter (1978). Purpose of the experiment is to find the optimal settings for reaction time, reaction temperature and the catalyst amount that maximize the percent conversion of polymer (Y_1) with a lower bound 80 and achieve a target value of 57.5 for the thermal activity (Y_2). A lower bound of 55 and an upper bound of 60 are set for thermal activity.

- Reaction time in minutes (x_1)
- Reaction temperature in $^{O}\mathrm{C}$ (x_2)
- Catalyst in % (x_3)

The prediction equations for the responses are found as the following after the use of central composite design model;

$$Y_1 = 81.09 + 1.03x_1 + 4.04x_2 + 6.20x_3 - 1.83x_1^2 + 2.94x_2^2 - 5.19x_3^2 \\ + 2.13x_1x_2 + 11.37x_1x_3 - 3.87x_2x_3$$

$$Y_2 = 60.5 + 3.58x_1 + 2.23x_3$$

The optimal solution by desirability functions yields to following result from equation (2) with $s = t = 1$ and equivalent importance setting $k_1 = k_2$ for each response. Response surface plot of the factors against overall desirability is illustrated in Figure 4 where catalyst set at -0.56.

$$x_1 = -0.49 \qquad x_2 = 1.68 \qquad x_3 = -0.56$$
$$Conversion = 95.175 \qquad Thermal\ Activity = 57.50$$
$$Overall\ Desirability = 0.871$$

Figure 4. 3D Response Surface Plot

To initiate the sensitivity analysis, lower and upper edge values are assigned for importance, weight and range of each response as given in Table 1. For both of the responses, importance parameter is varied on scale between 1 and 5 and weight is varied between 0.5 and 2 where the first becomes the lower edge and latter is the upper edge that the sensitivity is being evaluated. Sensitivity on the range of the responses is evaluated with respect to the size of the specification band of each response.

Table 1. Parameter edge values for sensitivity analysis

All of the three parameters are varied on 2-levels for each response and a fractional factorial design is established. In order to maintain efficiency, a fractional design with 6 factors and 16 runs is chosen. Following the levels of each of these parameters, individual desirabilities and the corresponding overall desirability is evaluated at each run. This overall desirability has now become the new response value that is going to be used in obtaining the prediction equation.

Importance of conversion of polymer, $k_1 \rightarrow$ A

Importance of thermal activity, $k_2 \rightarrow$ B

Weight of conversion of polymer, $s_1 \rightarrow$ C

Weight of thermal activity, $s_2 = t_2 \rightarrow$ D

Range of conversion of polymer, $\left(\max_{c.polymer} - LSL_{c.polymer}\right) \rightarrow$ E

Range of thermal activity, $\left(USL_{t.activity} - LSL_{t.activity}\right) \rightarrow$ F

Experimental design setup given in Table 2 is analysed by Design-Expert® software and the resulting ANOVA is given in Table 3. Prediction equation on the overall desirability is found as following.

$$\textit{Overall Desirability} = 0.68 + 0.026(\mathrm{A}) + 0.004(\mathrm{B}) - 0.056(\mathrm{C}) - 0.069(\mathrm{D}) + 0.23(\mathrm{E}) + 0.071(\mathrm{F})$$

Overall desirability model is found to be significant with a p-value $<< 0.05$ and an acceptable R-square value. It can be observed that range of conversion is the most sensitive parameter where importance parameter of thermal activity is the least sensitive one. Others have relatively similar sensitivities. Any increase in the range of conversion will increase the overall desirability rapidly. Notice that, optimal levels of the input variables achieved from several design points (e.g. runs 2, 10, 11, 12 and 13) ended up with equal settings with different overall desirability levels which proves the importance of the sensitivity analysis on overall desirability. In the solution space, a high and a low overall desirability might end up with the same solution settings and this does not necessarily make one solution better than the other.

Table 2. DOE setup for sensitivity analysis

Table 3. Design-Expert® ANOVA output

6. Conclusions

Sensitivity analysis is important in order to understand the accuracy of information at hand, to explore the effect of decision maker's uncertainty about the priorities of the process or product and to identify the values of parameters and responses in multiresponse optimization. The desirability functions approach, which has found a great deal of interest both from practitioners and researchers, has been used intuitively with respect to its defining parameters. This paper proposes and illustrates a sensitivity analysis procedure that is utilized by the help of experimental design tools. The proposed procedure identifies the effect of importance, weight and range parameters of each response on the overall desirability by using the coefficients of prediction equation obtained from the design of the various settings of the very same parameters. This experimental setup is built and solved by the classical factorial design or by fractional factorial whereas the number of competing responses is high and design resources are scarce.

Previous attempts of evaluating trade-offs in the desirability functions focuses on the calculation of marginal rates of substitution between conflicting responses. Taking another step further to analyze the effect of each building structure of these functions on the unifying objective function, overall desirability, is a crucial task. As has been mentioned before, the example we solved is a heavily used benchmark problem for the introduction and comparison of new techniques within the multiresponse optimization literature. The optimal settings for maximizing the conversion of polymer and achieving a nominal value for thermal activity heavily relied on the width of the specification band. Lack of a common consensus for the choice of this bandwidth makes sensitivity analysis inevitable. More importantly, such an analysis will help to identify the factors that need improvement towards achieving a better optimal solution. Practitioners should keep in mind that a higher overall desirability does not necessarily mean a better solution since the manipulation of overall desirability is quite possible by simply varying parameter values. Enforcing certain edge values or gathering a higher order prediction model (to see the interactions between parameters) will further motivate the initiation of sensitivity analysis to incorporate the subjective nature of parameter selection.

Other multiresponse optimization techniques that use the unifying objective approach may also benefit from the proposed sensitivity analysis procedure. Future research may expand the application on such methods.

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Table 1. Parameter edge values for sensitivity analysis

			Importance			Weight			Range	
			Min	*Max*		*Min*	*Max*		*Min*	*Max*
Response 1 (Conversion)	Actual	A	1	5	C	0.5	2	E	95-100	65-100
	Coded		-1	1		-1	1		-1	1
Response 2 (Thermal Activity)	Actual	B	1	5	D	0.5	2	F	55-60	50-65
	Coded		-1	1		-1	1		-1	1

Table 2. DOE setup for sensitivity analysis

Run	***Coded Settings***						***Desirability***	***Matching values for Responses and input variables***				
	A	***B***	***C***	***D***	***E(ABC)***	***F(BCD)***		***reaction time***	***reaction temp.***	***catalyst***	***Conversion***	***Thermal Activity***
1	-1	-1	-1	-1	-1	-1	0.443	-0.68	1.68	-0.73	95.33	56.46
2	1	-1	-1	-1	1	-1	0.940	-0.49	1.68	-0.56	95.18	57.50
3	-1	1	-1	-1	1	1	0.988	-0.49	1.68	-0.57	95.18	57.50
4	1	1	-1	-1	-1	1	0.702	-1.41	1.68	-1.28	98.50	52.60
5	-1	-1	1	-1	1	1	0.862	-0.49	1.68	-0.56	95.18	57.50
6	1	-1	1	-1	-1	1	0.878	-1.59	1.68	-1.45	100.00	51.58
7	-1	1	1	-1	-1	-1	0.319	-0.29	1.68	-0.41	95.33	58.58
8	1	1	1	-1	1	-1	0.862	-0.49	1.68	-0.56	95.18	57.50
9	-1	-1	-1	1	-1	1	0.454	-0.88	1.68	-0.87	95.78	55.42
10	1	-1	-1	1	1	1	0.940	-0.49	1.68	-0.56	95.18	57.50
11	-1	1	-1	1	1	-1	0.988	-0.49	1.68	-0.56	95.18	57.50
12	1	1	-1	1	-1	-1	0.433	-0.49	1.68	-0.56	95.18	57.50
13	-1	-1	1	1	1	-1	0.862	-0.49	1.68	-0.56	95.18	57.50
14	1	-1	1	1	-1	-1	0.026	-0.91	1.68	-0.89	95.86	55.28
15	-1	1	1	1	-1	1	0.319	-0.78	1.68	-0.79	95.51	55.96
16	1	1	1	1	1	1	0.862	-0.49	1.68	-0.56	95.18	57.50

Table 3. Design Expert® output

Response: Overall Desirability

Analysis of variance table [Partial sum of squares]

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F	
Model	1.088	6	0.181	6.129	0.008	significant
A	0.010	1	0.010	0.354	0.567	
B	0.000	1	0.000	0.009	0.926	
C	0.050	1	0.050	1.698	0.225	
D	0.077	1	0.077	2.602	0.141	
E	0.870	1	0.870	29.404	0.0004	
F	0.080	1	0.080	2.711	0.134	
Residual	0.266	9	0.030			
Cor Total	1.355	15				

Std. Dev.	0.172	R-Squared	0.803
Mean	0.680	Adj R-Squared	0.672
C.V.	25.305	Pred R-Squared	0.379
PRESS	0.842	Adeq Precision	7.171

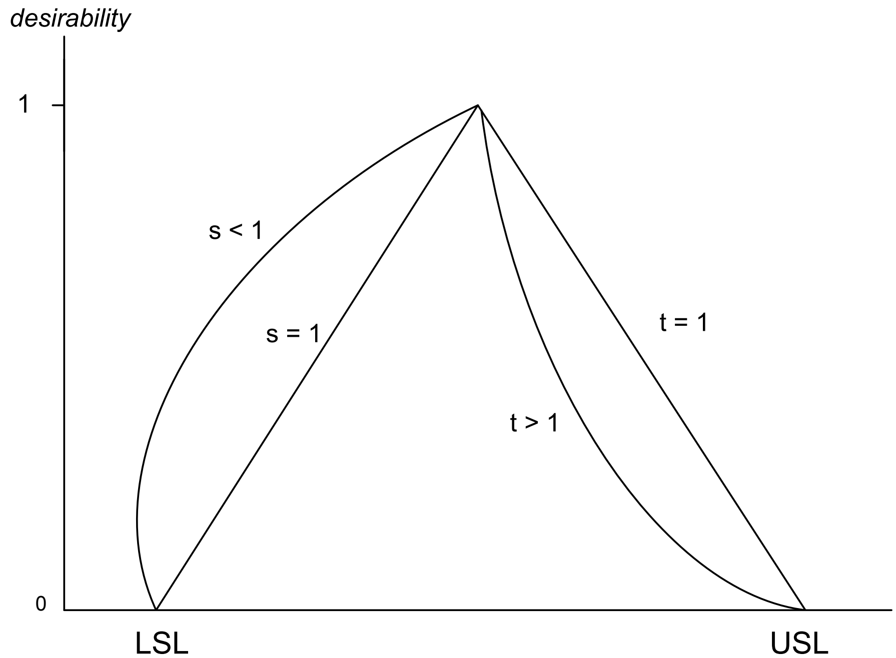
Factor	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High	VIF
Intercept	0.680	1	0.043	0.583	0.777	
A-A	0.026	1	0.043	-0.072	0.123	1
B-B	0.004	1	0.043	-0.093	0.101	1
C-C	-0.056	1	0.043	-0.153	0.041	1
D-D	-0.069	1	0.043	-0.167	0.028	1
E-E	0.233	1	0.043	0.136	0.330	1
F-F	0.071	1	0.043	-0.026	0.168	1

Figure 1. Nominal the best desirability function

Figure 2. Smaller the better desirability function

Figure 3. Larger the better desirability function

Figure 4. 3D Response Surface Plot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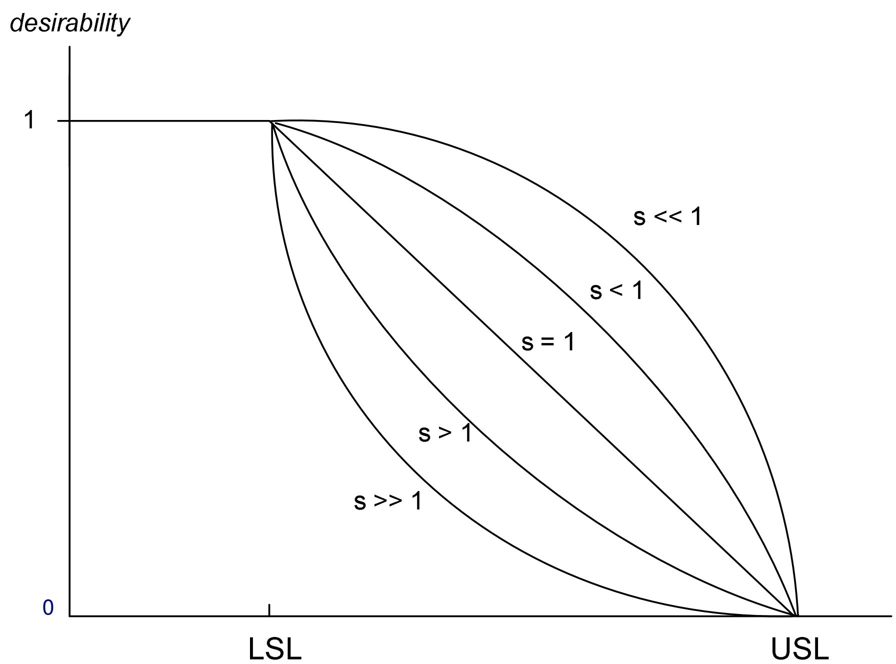
0
s < 1
s = 1
t = 1
t > 1
LSL
USL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s > 1
s >> 1
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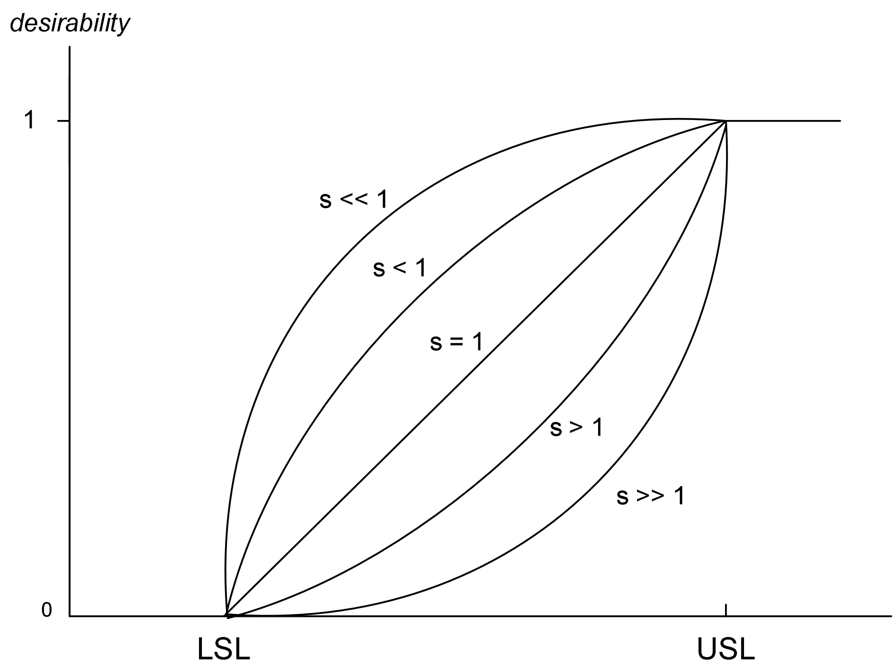
LSL
USL


desirability
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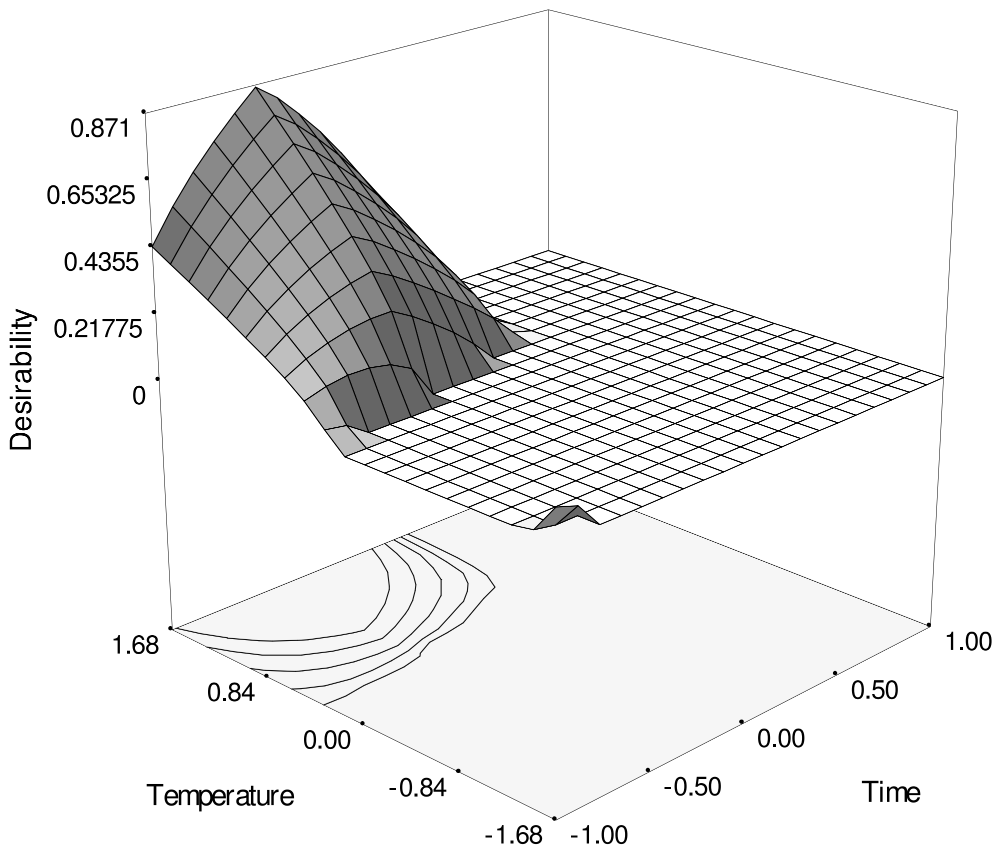
LSL
USL



Desirability
0.871
0.65325
0.4355
0.21775
0
Temperature
1.68
0.84
0.00
-0.84
-1.68
Time
-1.00
-0.50
0.00
0.50
1.00