Optimization in Multiple Response Model with Modified Desirability Function*

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Abstract

The desirability function approach to multiple response optimization is a useful technique for the analysis of experiments in which several responses are optimized simultaneously. But the existing methods have some defects, and have to be modified to some extent. This paper proposes a new method to combine the individual desirabilities.

Key Words: Response Surface, Multiple Responses, Optimization, Desirability Function, Harmonic Average

1. Introduction

Response surface methodology (RSM) consists of a group of techniques used in the empirical study of the relationship between the response and a number of input variables. Consequently, the experimenter attempts to find the optimal setting for the input variables that optimize the response. Most of the work in RSM has been focused on the case where there is only one response of interest. But in most experiments there are several responses of interest. The desirability function approach to multiple response optimization is a useful technique for the analysis of experiments in which several responses have to be optimized simultaneously. Originally developed by Harrington (1965) and later modified by Derringer and Suich (1980), the desirability function approach is one of the most frequently used multiresponse optimization techniques in practice (Derringer (1994)).

This paper proposes a new method to combine the individual desirabilities. In Section 2,

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there will be a review of literature about desirability function. In Section 3, we will introduce the modification of overall desirability function. And in Section 4, there will be examples about the proposed method.

2. Desirability Function

In many experimental situations, it is quite common for several responses, rather than a single response, to be measured for each setting of a group of input variables. Multiresponse optimization is the most visible and important aspect of multiresponse analysis. The object is to determine conditions on the input variables $x_1, x_2, \cdots, x_k$ that lead to optimal, or nearly optimal, values of the response variables, $y_1, y_2, \cdots, y_m$ There are several approaches to multiresponse optimization. Desirability function method is the one approach of those.

Derringer and Suich (1980) introduced the concept of desirability, whereby each response function is transformed into a desirability function. The choice of these transformations is subjective as it is governed by the experimenter's assessment of the importance of each response. A measure of the overall desirability of the response is obtained by using the geometric mean of the individual desirability functions. The geometric mean is then maximized over the region of interest.

The desirability function involves transformation of each estimated response variable $\hat{y}_i$ to a desirability value d_i, where $0 \le d_i \le 1$ The value of d_i increases as the "desirability" of the corresponding response increases.

Consider the case when the characteristic of interest is larger-the-better. Let $d_i(x)$ be the i th individual desirability function, which is usually defined by

$$d_i(x) = \begin{cases} 0 & \hat{y}_i(x) \le y_{i^*} \\ [\frac{\hat{y}_i(x) - y_{i^*}}{y_i^* - y_{i^*}}]^r & y_{i^*} < \hat{y}_i(x) < y_i^* \\ 1 & \hat{y}_i(x) \ge y_i^* \end{cases}$$

where y_{i*} is the minimum allowable value of $\hat{y}_i(x)$, y_i^* is the satisfactory value of $\hat{y}_i(x)$ for $i = 1, 2, \cdots, m$, and r is an arbitrary positive constant.

If the characteristic is smaller-the-better, the individual desirability function $d_i(x)$ is usually defined by

$$d_i(x) = \begin{cases} 1 & \hat{y}_i(x) \le y_{i^*} \\ [\frac{y_i - \hat{y}_i(x)}{y_i^* - y_{i^*}}]^r & y_{i^*} < \hat{y}_i(x) < y_i^* \\ 0 & \hat{y}_i(x) \ge y_i^* \end{cases}$$

where y_{i^*} is the satisfactory value of $\hat{y}_i(x)$, y_i^* is the maximum allowable value of $\hat{y}_i(x)$ for $i=1,\ 2,\ \cdots, m$

If the characteristic is nominal-is-best, the individual desirability function is defined by

$$d_i(x)=\begin{cases}[\dfrac{\hat{y}_i(x)-y_{i^*}}{t_i-y_{i^*}}]^s & y_{i^*}\le \hat{y}_i(x)\le t_i\\ [\dfrac{\hat{y}_i(x)-y_i^*}{t_i-y_i^*}]^c & t_i<\hat{y}_i(x)<y_i^*\\ 0 & \hat{y}_i(x)<y_{i^*}\text{ or }\hat{y}_i(x)y_i^*\end{cases}$$

where t_i is the target value for the i th response, y_{i^*} is the minimum allowable value of $\hat{y}_i(x)$, y_i^* is the maximum allowable value of $\hat{y}_i(x)$, and s and c are arbitrary positive constants.

The individual desirabilities are then combined using the geometric mean,

$$D=(d_1\times d_2\times\ \cdots\ \times d_m)^{1/m} \tag{2.1}$$

This single value of D gives the overall assessment of the desirability of the combined response levels. Clearly, the range of D will fall in the interval [0,1] and D will increase as the balance of the properties becomes more favorable. D also has the property that if any $d_i=0$ (that is, if one of the response variables is unacceptable) then D = 0 (that is, the over-all product is unacceptable). It is for these reasons that the geometric mean, rather than some other function of the d_is such as the arithmetic mean, was used.

3. Modification of Overall Desirability Function

3.1 Existing Methods

The conditions of the overall desirability function D is,

Condition 1> If any d_i equals to 0 then D equals to 0, if all d_i equals to 1 the D equals to 1 and D is non-decreasing function.

Condition 2> D must increase as the balance of the properties becomes more favorable. For instance, D must be larger when d_is are (0.5, 0.5) than (0.4, 0.6)

The reason why the geometric mean was selected previously is that it is the most simple function satisfying these conditions. The geometric mean is described in (2.1).

The most important merit of geometric mean is that it's the most simple function satisfying that conditions using all d_is in calculation. But the geometric mean has some demerits. Firstly, since d_is are quadratic functions, D is a function of order 2*m. Therefore, if m is too large, there will be a problem in optimization. Secondly, the degree of satisfying the condition 2 is weaker than the "Maximin" approach (Kim and Lin, 2006) or the method which will be produced in this literature. And, the maximin approach is a substitute for the geometric mean. This method is described as,

$$D = \max[\min\{d_1(\hat{y_i}(x)), \cdots d_m(\hat{y_1}(x))\}] \tag{3.1}$$

The merits of this method are that it strongly satisfies the condition 2 and that the existence of dependency among responses does not affect this method and that it is intuitive and understandable. But this method has a serious demerit. It is that this method excludes any other d_is except the smallest d_i. For example, it cannot distinguish that d_is are (0.3,0.4,0.9) from that those are (0.3,0.3,0.3). And it prefers that d_is are (0.3, 0.3, 0.3) rather than that d_is are (0.29,0.9,1).

3.2 Proposed Method ; Harmonic Average Method

If we elaborate the condition 2, we can see that it's characteristic is similar to the method which Taguchi proposed in case of the large-the-better.

$$SN_i = 10\log(\frac{1}{n}\sum_{j=1}^{n}\frac{1}{y_{ij}^2}) \tag{3.2}$$

In the formula to compute the SN ratio in case of the large-the-better, if each value is large and if the dispersion is small, the SN ratio is large. So we firstly define D as,

$$D = -10\log(\frac{1}{m}\sum_{i=1}^{m}\frac{1}{d_i^2}) \tag{3.3}$$

If the d_i is zero, we regard the $1/d_i$ as an infinite value.

But multiplying by 10, taking log and dividing by m do not affect the optimization. So we simply define D as,

$$D = (\sum_{i=1}^{m}\frac{1}{d_i^2})^{-1} \tag{3.4}$$

And if all d_is are 1, we want that D is 1 also. So we multiply the formula by m.

$$D = m(\sum_{i=1}^{m}\frac{1}{d_i^2})^{-1} \tag{3.5}$$

And since the square of d_i complicates the computation, we remove the square term. So we finally define D as,

$$D=m(\sum_{i=1}^{m}\frac{1}{d_i})^{-1} \tag{3.6}$$

After converting the formula like this, it seems like a harmonic average form and this satisfies the condition 2 more strongly than the geometric mean. And this will be a good measure because this overcomes the demerit of the "Maximin" approach which doesn't use all d_is. In other words, this method will have a middle property between the geometric mean and the "Maximin" approach.

3.3 Weighted Optimization

It's a good idea to substitute $D=D(\frac{d_i}{w_i})$ for $D=D(d_i)$ Because, in a dependent variable which has a large weight, this method makes the d_i smaller which was small originally. And finally, this point will not be selected as an optimal point. In other words, the speed that the chance of being selected is decreasing is much faster than the speed that d_i is decreasing.

3.3.1 Weighted Geometric Mean

In case of the geometric mean, if we substitute $\frac{d_i}{w_i}$ for d_i we can obtain this form,

$$D=(w_1w_2\cdots w_m)^{1/m}(\frac{d_1d_2\cdots d_m}{w_2w_2\cdots w_m})^{1/m}=(d_1d_2\cdots d_m)^{1/m} \tag{3.7}$$

In fact, this form is exactly the same as the ordinary geometric mean.

3.3.2 Weighted Maximin Approach

In case of the maximin approach, if we substitute $\frac{d_i}{w_i}$ for d_i we can obtain this form,

$$D=\max(w_i)\min[\frac{d_1}{w_1},\frac{d_2}{w_2},\cdots\frac{d_m}{w_m}] \tag{3.8}$$

So this method has a property that it seriously depends on the dependent variable which has a large weight.

3.3.3 Weighted Harmonic Aaverage

In case of the harmonic average, if we substitute $\frac{d_i}{w_i}$ for d_i we can obtain this form,

$$D=\sum_{k=1}^{m} w_k(\sum_{i=1}^{m}\frac{w_i}{d_i}) \tag{3.9}$$

This method has a good form and it does not seem that it has a bad property. So this method is the best among the three methods.

3.4 Graphical Approach for Response Optimization

In the optimized point, it is an important property in practice that the overall desirability value decreases slowly as one independent variable varies a little when the other independent variables are fixed. So, if a new method is proposed we must check that the method has that property. But, it is difficult to check that property by using a theoretical method. So, we will check it by using R graphics in Section 5. The conclusion is that our proposed method, harmonic average method, has that property more than the existing methods in many cases.

4. Example

4.1 Example. Colloidal gas Aphrons (CGA) Study

A real problem with multiple responses reported in the chemical engineering literature (Jauregi *et al.*, 1997) is employed to demonstrate the use of the existing multiresponse optimization approaches. The same example will be used later to illustrate the proposed approach. When surfactant solutions are mixed at high speeds, micro bubbles (10-100 μm in diameter) are formed. It is postulated that these bubbles, calledcolloidal gas aphrons (CGAs), are composed of a gaseous inner core surrounded by a thin soapy film. The properties of the CGAs are measured by three different responses-stability(y_1), volumetric ratio (y_2), and temperature (y_3). The responses, y_1, y_2, and y_3 are larger-the-better(LTB), smaller-the-better(STB) and nominal-the-best(NTB) type responses, respectively. The purpose of the experiment was to determine the effects of concentration of surfactant (x_1), concentration of salt (x_2) and time of stirring (x_3) on the CGA properties.

The experiment was conducted in a central composite design with eight factorial points, six axial points and a center point. The center point was replicated six times and the other design points were replicated twice. The dataset is displayed in Table 1.

In Table 2, the "Maximin" approach does not consider the experimental point which has a small d_i and the geometric mean put relative importance on a point which has one big d_i. But the proposed method has a middle property between those methods.

Let us introduce the graphics mentioned in Section 3.4. The other independent variables are fixed on optimized points (if necessary, we can fix them to arbitrary points).

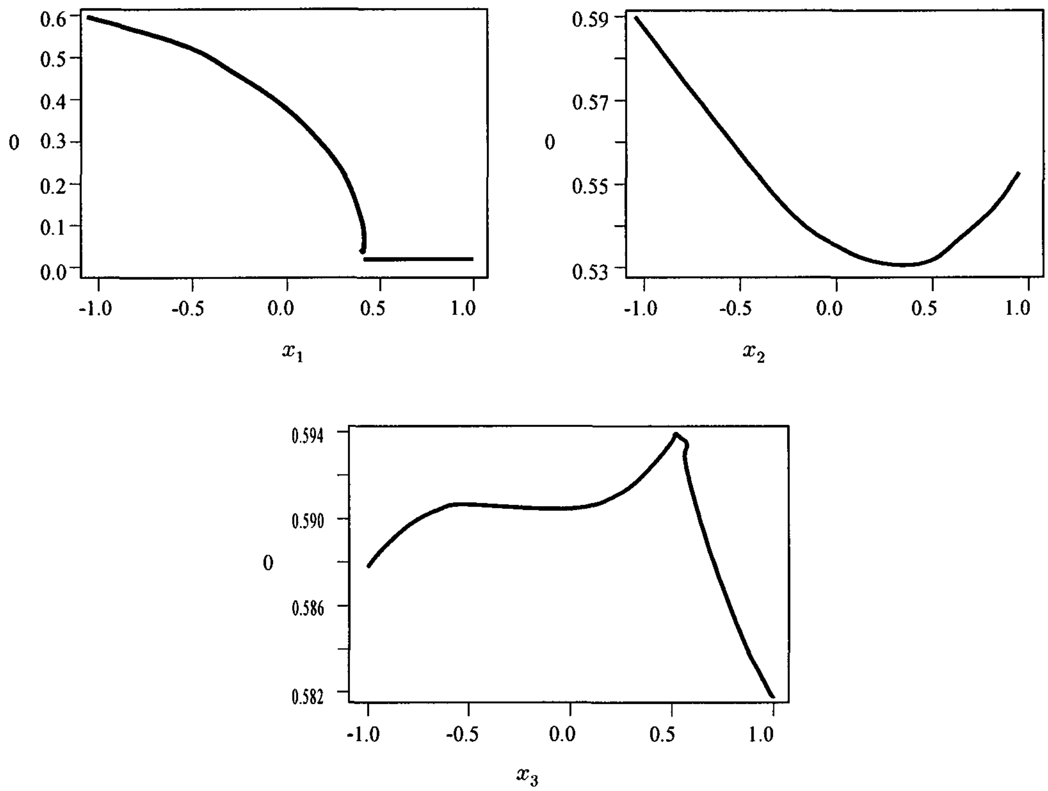

Figure 1. Geometric mean. method

In this example, the harmonic average method has the best property among the three methods since the overall desirability value decreases slowly as one independent variable varies a little around the optimum.

Next, we want to see the effect of the case that one response variable has an increasing weight.

We can see that d_1 is increasing so fast and d_2 is decreasing so fast as w_1 is increasing. In other words, this method has a property that it seriously depends on the dependent variable which has a large weight.

Table 1. The CGA study data 「Kim and Lin, 2006」

U	x_1	x_2	x_3	Rep.	y_1	y_2	y_3
1	-1	-1	-1	1	4.5	0.17	29
	-1	-1	-1	2	4.5	0.26	23
2	1	-1	-1	1	6.04	0.5	23
	1	-1	-1	2	6.39	0.53	25.4
3	-1	1	-1	1	3.81	0.17	22
	-1	1	-1	2	4.09	0.2	27
4	1	1	-1	1	5.67	0.44	25.5
	1	1	-1	2	5.19	0.4	21
5	-1	-1	1	1	4.67	0.32	20
	-1	-1	1	2	4.22	0.32	41
6	1	-1	1	1	6.73	0.57	35.5
	1	-1	1	2	6.57	0.57	18
7	-1	1	1	1	3.4	0.12	43
	-1	1	1	2	4.32	0.28	20
8	1	1	1	1	5.72	0.46	19
	1	1	1	2	5.09	0.5	34
9	-1	0	0	1	4.09	0.27	36
	-1	0	0	2	4.38	0.23	24
10	1	0	0	1	5.52	0.52	30
	1	0	0	2	5.39	0.51	24
11	0	-1	0	1	5.92	0.61	32
	0	-1	0	2	5.93	0.59	23.4
12	0	1	0	1	4.74	0.36	36
	0	1	0	2	4.5	0.3	21
13	0	0	-1	1	5.01	0.36	27
	0	0	-1	2	4.7	0.25	24
14	0	0	1	1	4.94	0.53	38
	0	0	1	2	5.01	0.51	25
15	0	0	0	1	4.85	0.47	34
	0	0	0	2	4.94	0.46	34
	0	0	0	3	4.98	0.49	33
	0	0	0	4	4.89	0.48	24
	0	0	0	5	4.94	0.46	19
	0	0	0	6	5.01	0.47	25

Notes) U is a design point number. x_1, x_2 and x_3 are coded values. Measurement units for y_1, y_2, y_3 are as follows: y_1=log(seconds), y_2=none(ratio), y_3=°C. y_{uj} is the response data of y_j at the uth design point, j=1,2,3; u=1,...,15.

Table 2. Results

	G.M	S.N.	M.A.	H.A.
D	0.5943461	0.317624	0.5098694	0.5724967
x_1	-0.997241	-0.681172	-0.519439	-0.757084
x_2	-0.995765	-0.996792	-0.979151	-0.998316
x_3	0.5349995	-0.984887	-0.996745	-0.993563
d_1	0.409971	0.4732917	0.5098694	0.4533545
d_2	0.512114	0.57629	0.5098848	0.6148699
d_3	0.9999965	0.7124896	0.7104982	0.7101946
$\hat{y}_1$	4.6398838	4.8931668	5.0394774	4.8134179
$\hat{y}_2$	0.343943	0.311855	0.3450576	0.2925651
$\hat{y}_3$	29.999947	25.687343	25.657473	25.652918

G.M. : geometric mean S.N. : Exp((SN ratio in large-the-better case)/10)

M.A. : Maximin approach H.A. : harmonic average

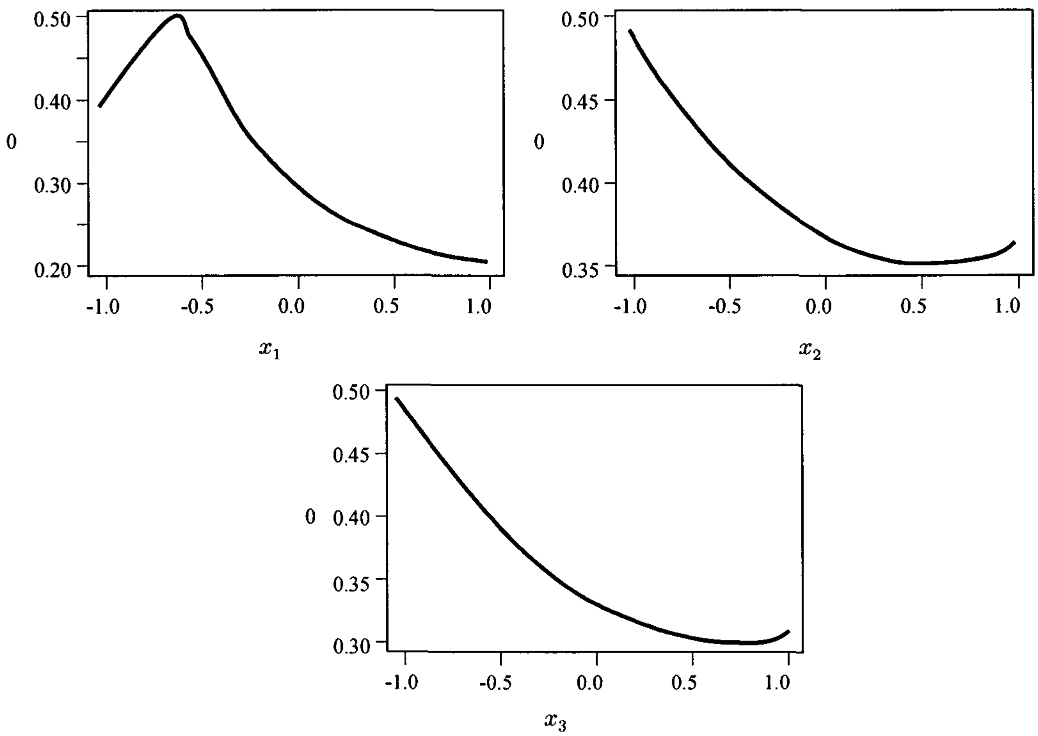

Figure 2. Maximin approach method

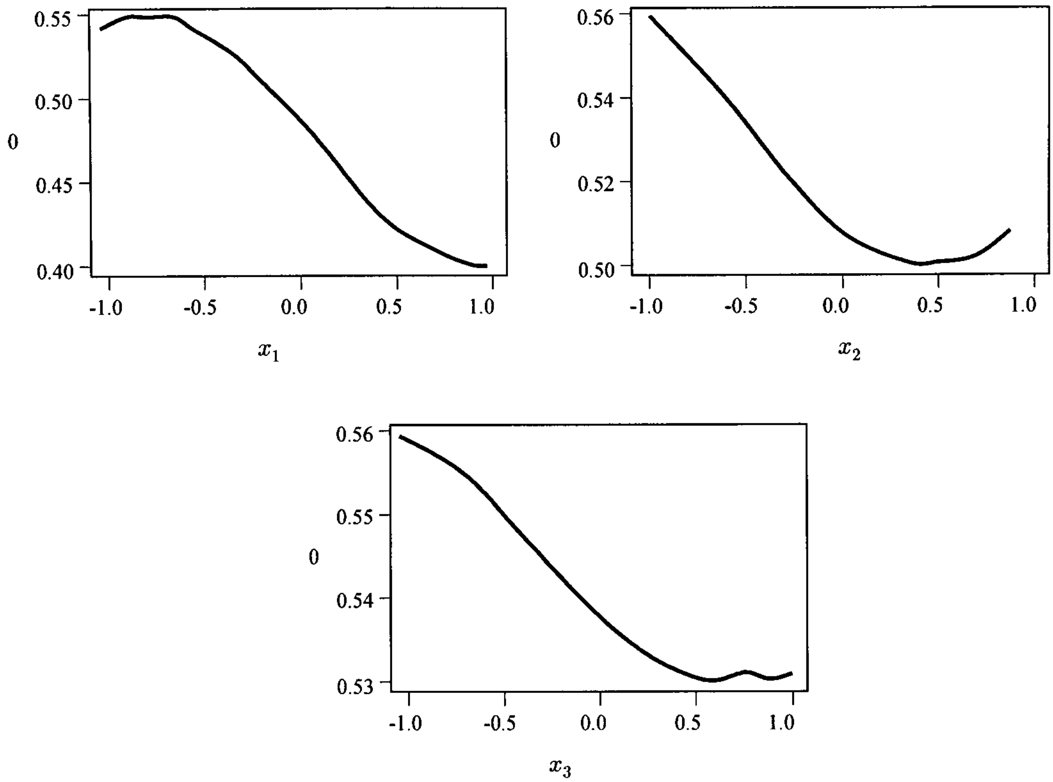

Figure 3. Harmonic average method

Table 3. Weighted maximin approach

$w = (w_1, w_2, w_3)$	d_1	d_2	d_3
(1,1,1)	0.509854	0.509858	0.7125
(2,1,1)	0.629037	0.315754	0.701114
(3,1,1)	0.725201	0.241718	0.641173
(4,1,1)	0.800103	0.200038	0.62057
(5,1,1)	0.821959	0.164393	0.631311
(6,1,1)	0.827888	0.137985	0.647073
(7,1,1)	0.83454	0.119223	0.656665
(8,1,1)	0.834729	0.10435	0.668515
(9,1,1)	0.842223	0.093594	0.671277
(10,1,1)	0.845082	0.084534	0.676463

Table 4. Weighted harmonic average

$w=(w_1, w_2, w_3)$	d_1	d_2	d_3
(1,1,1)	0.452393	0.614196	0.71275
(2,1,1)	0.527282	0.484541	0.708457
(3,1,1)	0.571917	0.412876	0.705379
(4,1,1)	0.605159	0.363452	0.700174
(5,1,1)	0.632867	0.327278	0.69477
(6,1,1)	0.731915	0.241327	0.636597
(7,1,1)	0.753237	0.227545	0.632747
(8,1,1)	0.772724	0.215886	0.628075
(9,1,1)	0.788766	0.206035	0.624197
(10,1,1)	0.804721	0.198087	0.618707

In case of the weighted maximin approach, (d_2, d_2) is (0.8,0.2) when w_1 is just 4, but in case of the weighted harmonic average, (d_2, d_2) is (0.8,0.2) when w_1 is just 10. That is, weighted harmonic average method doesn't seriously depend on the response variable which has the largest weight differently from the weighted maximin approach.

5. Concluding Remarks

This paper proposed the harmonic average method to combine the individual desirabilities. When we want to compute the overall desirability D, if we use the harmonic average method then it satisfies the condition 2 more strongly than the geometric mean method, and it will be a good measure because it overcomes the demerit of the maximin approach which doesn't use all d_is. Especially, if the response variables have weights depending on importance, using the harmonic average method is desirable.

Since we meet multiple response optimization problems frequently in practice, the harmonic average method which was proposed in this paper can be usefully employed. Such optimization method also can be implemented well for project activities in Six Sigma management.

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