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Optimal Designs Technique for Solving Unconstrained Optimization Problems with Univariate Quadratic Surfaces

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Abstract The author presented a new approach for solving unconstrained optimization problems having univariate quadratic surfaces. An illustrative example using this technique shows that an optimizer could be reached in just one move which compares favorably with other known ones, say, Fibonacci Search technique.

Keywords Fibonacci search technique, Unconstrained optimization, Response surface, Modified super convergent line series algorithm, Optimal designs of experiment

1. Introduction

In this paper, an alternative technique for solving unconstrained optimization problems with univariate quadratic surfaces is proposed. In real life, only very few problems exist where managers are concerned with taking decisions involving only one decision variable and without constraints. However, the justification for the study of such problems stem from the fact that it forms the basis of simple extensions and plays a key role to the development of a general multivariate algorithms as stated in [1] and [2].

According to [3], there are many iterative techniques for solving first unconstrained nonlinear problems and these techniques usually require many iterations of very tedious computations. Fibonacci Search and Golden Section Search techniques are some of the direct search techniques in this group that are used for finding the optimum of an arbitrary unimodal unconstrained univariate response function. The idea here is to identify the interval of uncertainty containing this optimum and the computational efforts involved in the two techniques which seek to minimize the size of the interval are enormous. In the case of Fibonacci search technique, the search procedures depend on a numerical sequence known as Fibonacci numbers. This method successfully reduces the interval in which the optimum of an arbitrary nonlinear function must lie (See [1]). On the other hand, according to [4] and [5], Golden Section Search technique is another traditional method used for finding the optimum of an arbitrary unimodal univariate objective function. The superiority of this technique over Fibonacci is that there is need for apriori specification of the resolution factor as well as the number of iterations before the Fibonacci technique is used. These are not necessary in Golden section technique as apriori specification of these might not be possible in practice, [6]. However, [7] had shown that Fibonacci Search technique is the best traditional technique for finding the optimal point for a single valued function. See also [8].

In order to circumvent these pitfalls, an alternative method for obtaining the required optimizer is of interest in this work which will later be generalized to accommodate response functions involving multi variables. The operation of the new algorithm makes use of the principles of optimal designs of experiment as can be seen in [9]. To design an experiment optimally, we select N support points within the experimental region such that optimal solution to the unconstrained optimization problems with univariate response surfaces could be realized. As by [10], a well-defined method to handle interactive effects in the case of quadratic surfaces has been provided. Since this new technique is a line search algorithm, it relies on a well-defined method of determining the direction of search as given by [11] which was a modification of [12]. See also [13]. This method seeks to determine the exact optimum of the unimodal unconstrained univariate response function rather than locating and reducing the interval where it lies which is the objective of the traditional methods. The algorithmic procedure which is given in the next section requires that the optimal support points that form the initial design matrix obtained from the entire experimental region be partitioned into r groups, r = 2, 3, … , n. However, [14] have shown that with r = 2, optimal solutions are obtained.

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2. Optimal Designs Technique

The sequential steps involved in this new method are given below.

Initialization: Let the response function, f(x) be defined as

$$f(x) = a_0 + a_1x + bx^2$$

Select N support points such that

$$3r \le N \le 4r \text{ or } 6 \le N \le 8$$

where r = 2 is the number of partitioned groups and by choosing N arbitrarily, make an initial design matrix

$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix}$$

Step 1: Compute the optimal starting point,

$$x_1^* = \sum_{m=1}^{N} u_m^* x_m^T,$$

where $u_m^* > 0$, $\sum_{m=1}^{N} u_m^* = 1$, $u_m^* = \frac{a_m^{-1}}{\sum a_m^{-1}}$, m = 1, 2, …, N, $a_m = x_m x_m^T$, m = 1, 2, …, N.

Step 2: Partition X into r = 2 groups and obtain

i. X_i, i = 1, 2.

ii. $M_i = X_i^T X_i$

iii. M_i^{-1}, i = 1, 2.

Step 3: Calculate the following:

(i) The matrices of the interaction effect of the x variable for the groups as

$$X_{1I} = \begin{bmatrix} x_{11}^2 \\ x_{12}^2 \\ \vdots \\ x_{1k}^2 \end{bmatrix} \text{ and } X_{2I} = \begin{bmatrix} x_{2(k+1)}^2 \\ x_{2(k+2)}^2 \\ \vdots \\ x_{2N}^2 \end{bmatrix}$$

where $k = \frac{N}{2}$.

(ii) Interaction vector of the response parameter, g = [b]

(iii) Interaction vectors, $I_i = M_i^{-1} X_i^T X_{iI}\, g$

(iv) Matrices of mean square error,

$$\bar{M}_i = M_i^{-1} + I_i I_i^T = \begin{bmatrix} \bar{v}_{i11} & \bar{v}_{i21} \\ \bar{v}_{i12} & \bar{v}_{i22} \end{bmatrix}$$

(v) Hessian matrices,

$$H_i = \text{diag}\left\{\frac{\bar{v}_{i11}}{\Sigma \bar{v}_{i11}}, \frac{\bar{v}_{i22}}{\Sigma \bar{v}_{i22}}\right\} = \text{diag}\{h_{i1}, h_{i2}\}$$

(vi) Normalized H_i as $H_i^* = \text{diag}\left\{\frac{h_{i1}}{\sqrt{\Sigma h_{i1}^2}}, \frac{h_{i2}}{\sqrt{\Sigma h_{i2}^2}}\right\}$

(vii) The average information matrix,

$$M(\xi_N) = \Sigma H_i^* M_i H_i^{*T} = \begin{bmatrix} \bar{m}_{11} & \bar{m}_{12} \\ \bar{m}_{21} & \bar{m}_{22} \end{bmatrix}$$

Step 4: Obtain

i. The response vector, $\mathbf{z} = \begin{bmatrix} z_0 \\ z_1 \end{bmatrix}$ where

$$z_0 = f(\bar{m}_{21}) \text{ and } z_1 = f(\bar{m}_{22})$$

ii. The direction vector, $\mathbf{d} = \begin{bmatrix} d_0 \\ d_1 \end{bmatrix} = M^{-1}(\xi_N)\mathbf{z}$

which gives $\mathbf{d^*} = d_1$

Step 5: Make a move to the point

$$x_2^* = x_1^* - \rho_1 \mathbf{d}^*$$

for a minimization problem or

$$x_2^* = x_1^* + \rho_1 \mathbf{d}^*$$

for a maximization problem where ρ_1 is the step length obtained from

$$\frac{df(x_2^*)}{d\rho_1} = 0$$

Step 6: Termination criteria. Is $|f(\mathbf{x_2^*}) - f(\mathbf{x_1^*})| < \varepsilon$ where $\varepsilon = 0.0001$?

i. Yes. Stop and set $\mathbf{x_2^*} = \mathbf{x}_{min}$ or $\mathbf{x}_{max.}$ as the case may be.

ii. No. Replace $\mathbf{x_1^*}$ by $\mathbf{x_2^*}$ and return to step 5. If $\rho_2 \cong 0$, then implement step 6(i).

3. Numerical Illustration

In this section, we give a numerical illustration of the optimal designs technique for solving unconstrained optimization problems with univariate quadratic surfaces. The example below gives such an illustration.

3.1. Example

$$\min f(x) = x^2$$

Solution

Initialization: Given the response function, $f(x) = x^2$ select N support points such that $3r \le N \le 4r$ or $6 \le N \le 8$ where r = 2 is the number of partitioned groups and by choosing N arbitrarily, make an initial design matrix

$$X = \begin{bmatrix} 1 & -1 \\ 1 & -0.5 \\ 1 & 0 \\ 1 & 0.5 \\ 1 & 1 \\ 1 & 1.5 \end{bmatrix}$$

Step 1: Compute the optimal starting point,

$x_1^* = \sum_{m=1}^{6} u_m^* x_m^T$, $u_m^* > 0$, $\sum_{m=1}^{6} u_m^* = 1$, $u_m^* = \frac{a_m^{-1}}{\sum a_m^{-1}}$, m = 1, 2, …, 6, $a_m = x_m x_m^T$, m = 1, 2, …, 6

$a_1 = [1 \quad -1]\begin{bmatrix} 1 \\ -1 \end{bmatrix} = 2, \ a_1^{-1} = 0.5,$

$a_2 = [1 \quad -0.5]\begin{bmatrix} 1 \\ -0.5 \end{bmatrix} = 1.25, \ a_2^{-1} = 0.8,$

$a_3 = [1 \quad 0]\begin{bmatrix} 1 \\ 0 \end{bmatrix} = 1, \ a_3^{-1} = 1,$

$a_4 = [1 \quad 0.5]\begin{bmatrix} 1 \\ 0.5 \end{bmatrix} = 1.25, \ a_4^{-1} = 0.8,$

$a_5 = [1 \quad 1]\begin{bmatrix} 1 \\ 1 \end{bmatrix} = 2, \ a_5^{-1} = 0.5,$

$a_6 = [1 \quad 1.5]\begin{bmatrix} 1 \\ 1.5 \end{bmatrix} = 3.25, \ a_6^{-1} = 0.3077$ and

$\sum a_m^{-1} = 3.9077.$

$u_1^* = \frac{0.5}{3.9077} = 0.1280, \ u_2^* = \frac{0.8}{3.9077} = 0.2047,$

$$u_3^* = \frac{1}{3.9077} = 0.2559,\ u_4^* = \frac{0.8}{3.9077} = 0.2047$$

$$u_5^* = \frac{0.5}{3.9077} = 0.1280,\ u_6^* = \frac{0.3077}{3.9077} = 0.0787.$$

Hence, the optimal starting point is

$$x_1^* = \sum_{m=1}^{6} u_m^* x_m^T = 0.1280\begin{bmatrix}1\\-1\end{bmatrix} + 0.2047\begin{bmatrix}1\\-0.5\end{bmatrix}$$

$$+ 0.2559\begin{bmatrix}1\\0\end{bmatrix} + 0.2047\begin{bmatrix}1\\0.5\end{bmatrix} + 0.1280\begin{bmatrix}1\\1\end{bmatrix}$$

$$+ 0.0787\begin{bmatrix}1\\1.5\end{bmatrix} = \begin{bmatrix}1\\0.1181\end{bmatrix}$$

Step 2: By partitioning X into 2 groups, we have the design matrices,

$$X_1 = \begin{bmatrix}1 & -1\\1 & -0.5\\1 & 0\end{bmatrix} \quad \text{and} \quad X_2 = \begin{bmatrix}1 & 0.5\\1 & 1\\1 & 1.5\end{bmatrix}$$

The information matrices are

$$M_1 = X_1^T X_1 = \begin{bmatrix}1 & 1 & 1\\-1 & -0.5 & 0\end{bmatrix}\begin{bmatrix}1 & -1\\1 & -0.5\\1 & 0\end{bmatrix}$$

$$= \begin{bmatrix}3 & -1.5\\-1.5 & 1.25\end{bmatrix}$$

and

$$M_2 = X_2^T X_2 = \begin{bmatrix}1 & 1 & 1\\0.5 & 1 & 1.5\end{bmatrix}\begin{bmatrix}1 & 0.5\\1 & 1\\1 & 1.5\end{bmatrix} = \begin{bmatrix}3 & 3\\3 & 3.5\end{bmatrix}$$

and their inverses are

$$M_1^{-1} = 0.6667\begin{bmatrix}1.25 & 1.5\\1.5 & 3\end{bmatrix} = \begin{bmatrix}0.8334 & 1.0001\\1.0001 & 2.0001\end{bmatrix} \text{ and}$$

$$M_2^{-1} = 0.6667\begin{bmatrix}3.5 & -3\\-3 & 3\end{bmatrix} = \begin{bmatrix}2.3335 & -2.0001\\-2.0001 & 2.0001\end{bmatrix}$$

Step 3 Calculate the following:

(i) The matrices of the interaction effect of the univariate for the groups as

$$X_{1I} = \begin{bmatrix}1\\0.25\\0\end{bmatrix} \quad \text{and} \quad X_{2I} = \begin{bmatrix}0.25\\1\\2.25\end{bmatrix}$$

(ii) Interaction vector of the response parameter,

$$g = [1]$$

(iii) Interaction vectors for the groups to be

$$I_1 = M_1^{-1} X_1^T X_{1I} g$$

$$= \begin{bmatrix}0.8334 & 1.0001\\1.0001 & 2.0001\end{bmatrix}\begin{bmatrix}1 & 1 & 1\\-1 & -0.5 & 0\end{bmatrix}\begin{bmatrix}1\\0.25\\0\end{bmatrix}[1]$$

$$= \begin{bmatrix}-0.1667 & 0.3334 & 0.8334\\-1 & 0 & 1.0001\end{bmatrix}\begin{bmatrix}1\\0.25\\0\end{bmatrix}$$

$$= \begin{bmatrix}-0.0834\\0.0001\end{bmatrix}$$

$$I_2 = M_2^{-1} X_2^T X_{2I} g$$

$$= \begin{bmatrix}2.3335 & -2.0001\\-2.0001 & 2.0001\end{bmatrix}\begin{bmatrix}1 & 1 & 1\\0.5 & 1 & 1.5\end{bmatrix}\begin{bmatrix}0.25\\1\\2.25\end{bmatrix}[1]$$

$$= \begin{bmatrix}1.3334 & 0.3334 & -0.6667\\-1.0001 & 0 & 1.0001\end{bmatrix}\begin{bmatrix}0.25\\1\\2.25\end{bmatrix}$$

$$= \begin{bmatrix}-0.8333\\2.0002\end{bmatrix}$$

(iv) Matrices of mean square error for the groups are

$$\bar{M}_1 = M_1^{-1} + I_1 I_1^T = \begin{bmatrix}0.8334 & 1.0001\\1.0001 & 2.0001\end{bmatrix}$$

$$+ \begin{bmatrix}-0.0834\\0.0001\end{bmatrix}\begin{bmatrix}-0.0834 & 0.0001\end{bmatrix}$$

$$= \begin{bmatrix}0.8334 & 1.0001\\1.0001 & 2.0001\end{bmatrix} + \begin{bmatrix}0.0070 & 0\\0 & 0\end{bmatrix}$$

$$= \begin{bmatrix}0.8404 & 1.0001\\1.0001 & 2.0001\end{bmatrix}$$

$$\bar{M}_2 = M_2^{-1} + I_2 I_2^T = \begin{bmatrix}2.3335 & -2.0001\\-2.0001 & 2.0001\end{bmatrix}$$

$$+ \begin{bmatrix}-0.8333\\2.0002\end{bmatrix}\begin{bmatrix}-0.8333 & 2.0002\end{bmatrix}$$

$$= \begin{bmatrix}2.3335 & -2.0001\\-2.0001 & 2.0001\end{bmatrix} + \begin{bmatrix}0.6944 & -1.6667\\-1.6667 & 4.0008\end{bmatrix}$$

$$= \begin{bmatrix}3.0279 & -3.6668\\-3.6668 & 6.0009\end{bmatrix}$$

(v) Matrices of coefficient of convex combinations of the matrices of mean square error are

$$H_1 = \text{diag}\left\{\frac{0.8404}{0.8404+3.0279}, \frac{2.0001}{2.0001+6.0009}\right\}$$

$$= \text{diag}\ \{0.2173, 0.2500\}$$

$$H_2 = I - H_1 = \text{diag}\ \{0.7827, 0.7500\}$$

and by normalizing H_i such that

$\Sigma H_i^* H_i^{*T} = I$, we have

$$H_1^* = \text{diag}\left\{\frac{0.2173}{\sqrt{0.2173^2 + 0.7827^2}}, \frac{0.2500}{\sqrt{0.2500^2 + 0.7500^2}}\right\}$$

$$= \text{diag}\{0.2675, 0.3162\}$$

$$H_2^* = \text{diag}\left\{\frac{0.7827}{\sqrt{0.2173^2 + 0.7827^2}}, \frac{0.7500}{\sqrt{0.2500^2 + 0.7500^2}}\right\}$$

$$= \text{diag}\{0.9636, 0.9487\}$$

(vi) The average information matrix is

$$M(\xi_N) = H_1^* M_1 H_1^{*T} + H_2^* M_2 H_2^{*T}$$

$$= \begin{bmatrix}0.2675 & 0\\0 & 0.3162\end{bmatrix}\begin{bmatrix}3 & -1.5\\-1.5 & 1.25\end{bmatrix}\begin{bmatrix}0.2675 & 0\\0 & 0.3162\end{bmatrix}$$

$$+ \begin{bmatrix}0.9636 & 0\\0 & 0.9487\end{bmatrix}\begin{bmatrix}3 & 3\\3 & 3.5\end{bmatrix}\begin{bmatrix}0.9636 & 0\\0 & 0.9487\end{bmatrix}$$

$$= \begin{bmatrix}0.2147 & -0.1269\\-0.1269 & 0.1250\end{bmatrix} + \begin{bmatrix}2.7856 & 2.7425\\2.7425 & 3.1502\end{bmatrix}$$

$$= \begin{bmatrix}3.0003 & 2.6156\\2.6156 & 3.2752\end{bmatrix}$$

Step 4 Obtain the response vector

$$\mathbf{z} = \begin{bmatrix}z_0\\z_1\end{bmatrix}$$

That is,

$z_0 = f(2.6156) = 2.6156^2 = 6.8414$

$z_1 = f(3.2752) = 3.2752^2 = 10.7269$

and hence, the direction vector

$$\mathbf{d} = \begin{bmatrix} d_0 \\ d_1 \end{bmatrix} = M^{-1}(\xi_N)\mathbf{z}$$

$$= \begin{bmatrix} 3.0003 & 2.6156 \\ 2.6156 & 3.2752 \end{bmatrix}^{-1} \begin{bmatrix} 6.8414 \\ 10.7269 \end{bmatrix}$$

$$= \begin{bmatrix} -1.8925 \\ 4.7872 \end{bmatrix}$$

which gives $\mathbf{d^*} = d_1 = 4.7872$

Step 5 Make a move to the point

$$x_2^* = x_1^* - \rho_1 d_1$$
$$= 0.1181 - 4.7872\rho_1$$

That is,

$$f(x_2^*) = (0.1181 - 4.7872\rho_1)^2$$
$$= 0.0139 - 1.1307\rho_1 + 22.9173\rho_1^2$$

and by derivative with respect to ρ_1, we have

$$\frac{df(x_2^*)}{d\rho_1} = -1.1307 + 45.8386\rho_1 = 0$$

which gives the step length as $\rho_1 = 0.0247$ and

$$x_2^* = x_1^* - \rho_1 d_1$$
$$= 0.1181 - 4.7872(0.0247)$$
$$= -0.0001.$$

Since $|f(\mathbf{x_2^*}) - f(\mathbf{x_1^*})| = |0 - 0.0139| = 0.0139 \neq \varepsilon$,

We make a second move to the point

$$x_3^* = x_2^* - \rho_2 d_1$$
$$= -0.0001 - 4.7872\rho_2$$

That is,

$$f(x_3^*) = (-0.0001 - 4.7872\rho_2{}^2$$
$$= 0 - 0.0010\rho_2 + 22.9173\rho_2^2$$

and by derivative with respect to ρ_2, we have

$$\frac{df(x_3^*)}{d\rho_2} = 0.0010 + 45.8386\rho_2 = 0$$

which gives the step length as $\rho_2 = -0.00002 \cong 0$. This means that the optimal solution was obtained at the first move and and hence,

$$x_2^* = = -0.0001 \cong 0 \text{ and } f(\mathbf{x_2^*}) = 0$$

This result is more efficient than that obtained by Fibonacci search technique which gave $x_{min} = (0.0472, -0.0184)$ and $f(x_{min}) = (0.0022, 0.0003)$.

4. Conclusions

We have successfully achieved the primary objective of this work by presenting an efficient alternative technique for solving unconstrained optimization problems having univariate quadratic surfaces. This was done by using the principles of optimal designs of experiment to show that the optimum could be obtained in just one move. A numerical illustration by this method which gave $x_2^* = -0.0001 \cong 0$ and $f(\mathbf{x_2^*}) = 0$ as the exact solution is more efficient than $x_2^* = (0.0472, -0.0184)$ and $f(x_2^*) = (0.0022, 0.0003)$ obtained from Fibonacci Search technique with several iterations.

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