Journal of Global Optimization **19:** 151–161, 2001.
© 2001 *Kluwer Academic Publishers. Printed in the Netherlands.*

Finding Global Minima with a Computable Filled Function

XIAN LIU
Department of Electrical and Computer Engineering, University of Alberta, Edmonton, Canada T6G 2G7 (e-mail: xliu@ee.ualberta.ca)

(Received 13 December 1999; accepted in revised form 30 October 2000

Abstract. The Filled Function Method is an approach to finding global minima of multidimensional nonconvex functions. The traditional filled functions have features that may affect the computability when applied to numerical optimization. This paper proposes a new filled function. This function needs only one parameter and does not include exponential terms. Also, the lower bound of weight factor a is usually smaller than that of one previous formulation. Therefore, the proposed new function has better computability than the traditional ones.

Key words: Filled function method, Global optimization, Gradient Methods, Nonlinear programming

1. Introduction

Studies on global optimization for non-convex nonlinear programming problems have been significantly accelerated since the two volumes named '*Towards Global Optimization*', edited by Dixon and Szegö ([3, 4]), were published. The recent progress in this field was reported by Horst and Tuy [10], Pardalos and Rosen [11], Törn and Žilinskas [13]. This paper concentrates on one of the approaches, the *Filled Function Method* (FFM). Early studies on the FFM can be found in [5, 6 and 9].

The FFM is an approach to find the global minimizer of a multimodal function $f(X)$ on R^n, under the following assumptions:

1. $f(X)$ is continuously differentiable;
2. $f(X)$ has only a finite number of minimizers; and
3. $f(X) \to +\infty$ as $\| X \| \to +\infty$.

Notice that the third assumption above implies the existence of a closed bounded domain $\Omega \subset R^n$ such that Ω contains all minimizers of $f(X)$ and the value of $f(X)$ when X is on the boundary of Ω is greater than any values of $f(X)$ when X is inside Ω. To introduce essentials of the FFM, let us define the following concepts:

DEFINITION 1.1. *A basin of $f(X)$ at an isolated minimizer X_1 is a connected domain B_1 which contains X_1 and in which starting from any point the steepest* *descent trajectory of* $f(X)$ *converges to* X_1*, but outside which the steepest descent trajectory of* $f(X)$ *does not converge to* X_1.

DEFINITION 1.2. *A hill of* $f(X)$ *at* X_1 *is the basin of* $-f(X)$ *at its minimizer* X_1*, if* X_1 *is a maximizer of* $f(X)$.

DEFINITION 1.3. *A local minimizer* X_2 *is said to be higher than* X_1 *if and only if* $f(X_2) > f(X_1)$*, and, for this case,* B_2 *is said to be a higher basin than* B_1*. In this paper,* B_h *and* B_l *denote all higher and lower basins than current basin* B_1 *of* $f(X)$*, respectively.*

DEFINITION 1.4. *A function* $P(X)$ *is called a filled function of* $f(X)$ *at* X_1 *if*

(1) X_1 *is a maximizer of* $P(X)$ *and the whole basin* B_1 *becomes a part of a hill of* $P(X)$*;*
(2) $P(X)$ *has no stationary points in any* B_h*s; and*
(3) There is a point X' *in a* B_l *(if such a basin exists) that minimizes* $P(X)$ *on the line through* X *and* X_1.

In this paper, we will allow an infinite maximizer of $P(X)$.

The FFM consists of two phases, local minimization and filling:

Phase 1: In this phase, a local minimizer X_1 of $f(X)$ is found. Any effective technique, for instance, the *variable metric method*, can be employed in phase one.

Phase 2: In this phase, an argumented function called the *filled function* is constructed. This function includes $f(X)$ in its formulation and has a maximizer at X_1. Furthermore, it has no stationary points in any B_hs, and does have a stationary point in a B_l. Phase 2 ends when such an X_s is found that X_s is in a B_l. Then, the FFM reenters phase 1, with X_s as the starting point, to find a new local minimizer X_2 of $f(X)$ (if such one exists), and so on.

The above process is repeated until the global minimizer is found.

Several filled functions have been proposed in the literature. Three popular ones are ([5, 6]):

$$P(X, r, \rho) = \exp(-\parallel X - X_1 \parallel^2 / \rho^2)/[r + f(X)] \tag{1}$$

$$G(X, r, \rho) = -\left\{\rho^2 \ln[r + f(X)] + \parallel X - X_1 \parallel^p\right\} \tag{2}$$

$$Q(X, a) = -[f(X) - f(X_1)] \exp(a \parallel X - X_1 \parallel^p) \tag{3}$$

where $p = 1$ or 2. r and ρ are adjustable parameters, and a is an adjustable positive weight factor. Both P and G-functions require two adjustable parameters, which need to be appropriately iterated and coordinated each other, hence their algorithmic realization is fairly complicated. For this reason, it is usually agreed that the Q-function is better than the other two, since it involves only one adjustable parameter. However, the Q-function includes an exponential term whose argument is the product of the weight factor a and the norm. As a becomes larger and larger, as required to preserve the filling property, the rapid increasing value of the exponential term will result in failure of computation even if the size of the feasible region is moderate. In practice, this kind of ill-conditioning problem frequently occurs. To make the Q-function work, many additional cares must be incorporated into the algorithm [8]. It is obvious that the exponential term in the Q-function has seriously limited its applicability to the practical global optimization problems, especially those raised from engineering.

In this paper, a new filled function, called the H-function, is proposed. We will show that the H-function is of superiority over previous ones. In Section 2, the H-function is defined and its filling property is proved. Then the computability of the H-function is discussed in Section 3. Next, in Section 4, an algorithm is presented. The results of numerical experiments for testing functions are reported in Section 5. Finally, conclusions are included in Section 6.

2. *H*-Function

The H-function is defined as:

$$H(X) = 1/\ln[1 + f(X) - f(X_1)] - a \parallel X - X_1 \parallel^2 \tag{4}$$

where a is a positive real used as the weight factor. Notice that, upon entering phase 2 of the FFM, $f(X) > f(X_1)$ has held already by the definition of X_1. Consequently, $f(X) > f(X_1) - 1$ and this ensures the existence of $H(X)$. During phase 2, the iteration process always checks the function value of current iteration point first. If at some X_s we obtain $f(X_s) < f(X_1)$, then X_s is in a lower basin than B_1 already. Phase 2 ends right at X_s and the FFM reenters phase 1 by starting from X_s.

The filling properties of $H(X)$ are exhibited by the following theorems.

THEOREM 2.1. *Given $d \in R^n$ and $f(X) > f(X_1)$, if*

$$d^T \nabla f(X) \geqslant 0, d^T(X - X_1) > 0 \tag{5}$$

or

$$d^T \nabla f(X) > 0, d^T(X - X_1) \geqslant 0 \tag{6}$$

then d is a descent direction of $H(X)$ at point X.

Proof. It follows from (4) that

$$d^T \nabla H(X) = -\left\{\frac{d^T \nabla f(X)}{[\ln(1 + f - f_1)]^2(1 + f - f_1)} + 2ad^T(X - X_1)\right\} \tag{7}$$

where $f - f_1$ stands for $f(X) - f(X_1)$ (throughout the following). Therefore, the conditions given guarantee $d^T \nabla H(X) < 0$. □

THEOREM 2.2. *Given* $f(X) > f(X_1)$, *and*

$$d^T \nabla f(X) < 0, d^T (X - X_1) > 0 \tag{8}$$

if

$$a > \frac{-d^T \nabla f(X)}{2d^T (X - X_1)[\ln(1 + f - f_1)]^2 (1 + f - f_1)} = a_l(X) \tag{9}$$

then d *is a descent direction of* $H(X)$ *at point* X.

Proof. Under the given conditions, the value of (7) is negative. □

THEOREM 2.3. *Given* $f(X) > f(X_1)$, *and*

$$d^T \nabla f(X) < 0, d^T (X - X_1) > 0 \tag{10}$$

if

$$a < a_l(X) \tag{11}$$

then d *becomes an ascent direction of* $H(X)$ *at point* X.

Proof. Under the given conditions, the value of (7) is positive. □

THEOREM 2.4. *It is possible that (11) holds.*

Proof. $a_l(X) \to +\infty$ as $f(X) > f(X_1)$ and $f(X) \to f(X_1)$, hence (11) holds. □

Now we give some remarks to the theorems presented above. The filling property of a filled function is mainly characterized by Theorems 2.1, 2.2 and 2.3. Theorem 2.1 exhibits that in the ascent region of the current basin (i.e., B_1) or a higher basin than B_1, d is always a descent direction of $H(X)$. Theorem 2.2 exhibits that in the descent region of a higher basin than B_1, d is still a descent direction of $H(X)$ provided that the weight factor a is sufficiently large. In other words, Theorems 2.1 and 2.2 together exhibit the desired filling property of $H(X)$. Furthermore, Theorems 2.3 and 2.4 indicate that, in a lower basin than B_1, d may become an ascent direction of $H(X)$ and this possibility does exist. Therefore, under the assumption that $f(X)$ is continuously differentiable, $H(X)$ must have a stationary point along d.

From its definition, the H-function appears more applicable to computational assignments, because (1) it does not include exponential terms; (2) it needs only one parameter. In addition, the lower bound of weight factor a is usually smaller than the case of Q-function (see Section 3).

3. Analysis on Weight Factor *a*

It has been described in Section 1 that the weight factor a plays a crux role in a filled function. Theoretically, the value of a must be sufficiently large to preserve a desirable filling capability. Computationally, the value of a should be small to make the numerical procedures healthy. Therefore, a filled function is a robust one if the value of $a_l(X)$ is small given a particular X. In this section, we compare the H-function with the Q-function in terms of the lower bound of a.

Let $d \in R^n$, then it follows from (3) that

$$d^T \nabla Q(X) = -\exp(\cdot)[d^T \nabla f(X) + 2a(f - f_1)d^T(X - X_1)] \tag{12}$$

where $\exp(\cdot)$ stands for $\exp(a \parallel X - X_1 \parallel^2)$. Consequently, with the same conditions as given in Theorem 2.2, if

$$a > \frac{-d^T \nabla f(X)}{2(f - f_1)d^T(X - X_1)} = a_q(X) \tag{13}$$

then d is a descent direction of $Q(X)$ at point X, because such an a satisfying (13) ensures that $d^T \nabla Q(X) < 0$.

Next, consider the ratio of $a_q(X)$ to $a_l(X)$:

$$a_q(X)/a_l(X) = [\ln(1 + f - f_1)]^2(1 + f - f_1)/(f - f_1) \tag{14}$$

It will be noted that (14) monotonically increases with argument $(f - f_1)$. Consequently, if $f - f_1 > 1.1$, then $a_l(X)$ is always less than $a_q(X)$. This implies that, even with a small weight factor a, the H-function preserves the desired filling property.

4. An Algorithm

We have seen that the weight parameter a plays a crucial role in filled functions. This parameter usually needs to be estimated through trial and error. It is possible, however, to develop a closed-form formula to update a if $X \in R^1$. In this case, (9) can be converted to the following form:

$$a = \frac{\xi \mid f'(X_s) \mid}{2 \mid X_s - X_1 \mid (1 + f - f_1)[\ln(1 + f - f_1)]^2} \tag{15}$$

where $f - f_1$ stands for $f(X_s) - f(X_1)$, $\xi > 1$, and subscript s corresponds to the termination point X_s of phase 2 in the last cycle.

The filling process works as follows: Initially, we set $a = a_0 > 0$. Suppose that this value of a is not large enough so that the termination point X_s is in a higher basin than B_1. In other words, at the end of phase 1 of the second cycle, a new local minimizer of $f(X)$, X_2, is found such that $f(X_2) > f(X_1)$. If so, we enter phase 2 again and use (15) to update the weight factor a and still repeat the same procedure of minimizing $H(X)$ as that in the first cycle. This time when iteration arrives to the X_s, (15) will make d a descent direction of $H(X)$.

In the rest of this section, we present an algorithm for unidimensional global optimization. The nomenclature in this algorithm is listed as follows:

D: the interval in which there is a global minimizer of $f(X)$ (Notice that D corresponds to domain Ω mentioned at the beginning of Section 1)
a: the weight factor in the formulation of the filled function
X_1: the found local minimizer of $f(X)$
f_1: the value of the objective function at X_1
X_1^0: the initial value of X_1, used for the iteration purpose. It is advisable to select one of the end points of D as X_1^0
f_1^0: the value of $f(X_1^0)$, used for the iteration purpose
X_0: the initial point to start phase 1 of the FFM
X_c: the initial point to start phase 2 of the FFM
δ: a small positive real number used to construct the starting point of phase 2

The algorithm is described as follows:

Step 0: Specify X_0, a, and D. $X_1^0 \to X_1$. $f_1^0 \to f_1$.
Step 1: Enter phase 1 of the FFM. Activate the minimization procedure to minimize the objective function $f(X)$, starting from X_0. Find a local minimizer $X_{\min}$. If $f(X_{\min}) \leqslant f_1$, then $X_{\min} \to X_1$ and $f(X_{\min}) \to f_1$; otherwise, use (15) to update a.
Step 2: Enter phase 2 of the FFM. $X_1 + \delta \to X_c$.
Step 3: Use X_1 and a to construct an H-function. Minimize this H-function with X_c as the starting point.
Step 4: Continue the down-hill search. Arrive at point X.
Step 5:
1. If X reaches the right end point of D, then $X_1 - \delta \to X_c$ and go to Step 3;
2. If X reaches the left end point of D, then taking the smallest minimum as the global one. Stop.
3. If $f(X) < f(X_1)$, then $X \to X_0$ and go to Step 1;
4. If X is a minimizer of the H-function, then $X \to X_0$ and go to Step 1;
5. Go to Step 4.

It should be emphasized that this algorithm does not weaken the deterministic attributes of the FFM, as in the case of $X \in R^1$ there are only two possible search directions, i.e., the positive and negative directions of the X-axis. For the multidimensional case, even $X \in R^2$, schemes based on probabilistic approaches to choose search directions for the filled function are needed, as Ge and Qin described in [5].

5. Numerical Experiments

The significance of a new optimization method depends after all on the effectiveness of solving practical problems. Several testing functions have been reported in the literature of global optimization. These functions are usually used to evaluate the numerical performance of a new approach. In this section, a set of well-recognized testing functions is described first, then the results of numerical experiment are presented.

5.1. TESTING FUNCTIONS

Six-hump camel-back ($n = 2$) [1]

$$f_C(X) = 4x_1^2 - 2.1x_1^4 + x_1^6/3 + x_1x_2 - 4x_2^2 + 4x_2^4 \quad (-3 \leqslant x_1, x_2 \leqslant 3)$$

The global minima are (0.08983, −0.7126) and (−0.08983, 0.7126).

Branin ($n = 2$) [2]

$$f_B(X) = (x_2 - 1.275x_1^2/\pi^2 + 5x_1/\pi - 6)^2 + 10(1 - 0.125/\pi)\cos(x_1) + 10 \quad (-5 \leqslant x_1 \leqslant 10, \quad 0 \leqslant x_2 \leqslant 15)$$

The global minima are (−3.142, 12.275), (3.142, 2.275), and (9.425, 2.425).

Goldstein-Price (G-P) ($n = 2$) [4]

$$f_G(X) = [1 + (x_1 + x_2 + 1)^2(19 - 14x_1 + 3x_1^2 - 14x_2 + 6x_1x_2 + 3x_2^2] \times [30 + (2x_1 - 3x_2)^2(18 - 32x_1 + 12x_1^2 + 48x_2 - 36x_1x_2 + 27x_2^2)] \qquad (-3 \leqslant x_1, x_2 \leqslant 3)$$

The global minimum is (0, −1).

Rastrigin ($n = 2$) [12]

$$f_R(X) = x_1^2 + x_2^2 - \cos(18x_1) - \cos(18x_2) \qquad (-1 \leqslant x_1, x_2 \leqslant 1)$$

This function has about 50 minima.
The global minimum is (0, 0).

Shubert III ($n = 2$) [6]

$$f_S(X) = \left\{\sum_{i=1}^{5} i \ \cos[(i+1)x_1 + 1]\right\}\left\{\sum_{i=1}^{5} i \ \cos[(i+1)x_2 + 1]\right\} + [(x_1 + 1.42513)^2 + (x_2 + 0.80032)^2 \qquad (-10 \leqslant x_1, x_2 \leqslant 10)$$

This function has 760 minima. The global minimum is (−1.42513, −0.80032). Because of the large number of local minima and the steep slope around the global

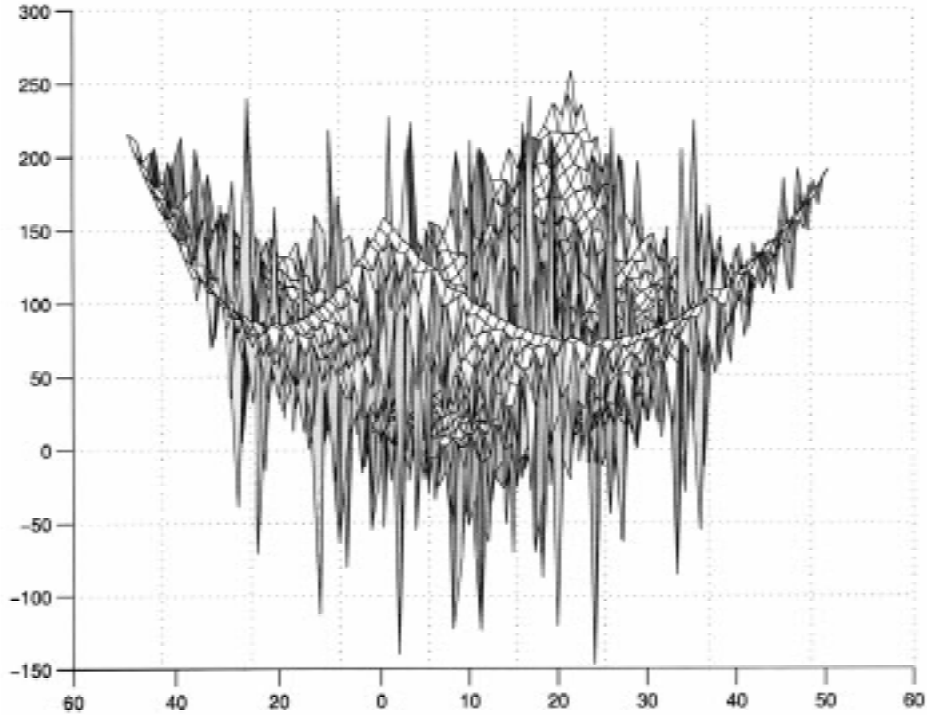

Figure 1. The Shubert function III.

minimum, the Shubert function III has widely been recognized as an important testing function. An illustration is given in Figure 1.

Sine-square I ($n = 6$) [7]

$$f_{sq1}(X) = \{10\sin^2(\pi x_1) + (x_n - 1)^2 + \sum_{i=1}^{n-1}(x_i - 1)^2[1 + 10\sin^2(\pi x_{i+1})]\}\pi/n \qquad (-10 \leqslant x_i \leqslant 10)$$

This function has about 60 minima.
The global minimum is (1, 1, 1, 1, 1, 1).

Sine-square II ($n = 6$) [7]

$$f_{sq2}(X) = \{10\sin^2(\pi y_1) + (y_n - 1)^2 + \sum_{i=1}^{n-1}(y_i - 1)^2[1 + 10\sin^2(\pi y_{i+1})]\}\pi/n$$

$$y_i = 1 + (x_i - 1)/4 \qquad (-10 \leqslant x_i \leqslant 10)$$

This function has about 30 minima.

Table 1. Numerical Experiments

	H-function		Q-function	
	K_f	K_t	K_f	K_t
Six-hump camel-back	137	281	204	346
Branin	97	252	97	3640
G-P	358	502	280	1059
Rastrigin	275	616	118	3589
Shubert III	395	558	NF	
Sine-square I	784	2387	NF	
Sine-square II	113	1716	NF	
Sine-square III	1350	4164	NF	

The global minimum is (1, 1, 1, 1, 1, 1).

Sine-square III ($n = 6$) [7]

$$f_{sq3}(X) = \{\sin^2(3\pi x_1) + (x_n - 1)^2[1 + \sin^2(2\pi x_n)] + \sum_{i=1}^{n-1}(x_i - 1)^2[1 + \sin^2(3\pi x_{i+1})]\}/10 \qquad (-10 \leqslant x_i \leqslant 10)$$

This function has about 180 minima.
The global minimum is (1, 1, 1, 1, 1, 1).

5.2. RESULTS OF NUMERICAL TESTING

To evaluate its effectiveness, the H-function has been used to seek the global minima of the testing functions described in the forgoing section. One of the representative traditional filled functions, the Q-function, has also been tested. Identical starting points were selected for both filled functions. The results of numerical experiments are presented in Table 1, where:

K_f – the total number of evaluations for the objective function and the filled function when the global minimizer was found
K_t – the total number of evaluations for the objective function and the filled function when the algorithm terminated
NF – failed to find the global minimizer

The evaluation of an algorithm or a formulation of the filled function may involve several layers of the concerned numerical procedures. It is believed, however, that the number of iterations should not be regarded as an appropriate index [7]. This is because, in the down-hill searching process, the number of iterations is dependent on what particular methods are used for the lower layers, such as unconstrained minimization or linear searching. Typically, there may be several function evaluations per iteration, and it is these evaluations that consume the major part of total execution time in practical problems. For this reason, we used the total number of evaluations of the objective function and the filled function as an appropriate measure for the performance of different filled functions. In terms of K_f and K_t, the results of numerical experiments presented in Table 1 imply that the H-function is superior to the Q-function, especially, for the complicated functions like the Shubert III function, or the high dimensional functions like the Sine-square functions. Consequently, it is reasonably to expect the H-function to be well applicable to the usually complicated engineering optimization models.

6. Conclusions

The Filled Function Method is an approach to find the global minimum of multimodal and multidimensional functions. Several filled function were reported in the literature. These traditional functions, however, may lack desired computability, due to either the exponential term or multiple parameters in their formulations. In addition, these functions may require a large weight factor to preserve the filling property. In numerical applications, all of these characteristics may lead to illness of computation.

In this paper, a new filled function called the H-function is proposed. This function requires neither exponential terms nor multiple parameters. Furthermore, the lower bound of weight factor a is usually smaller than that of one previous formulation. Therefore, the H-function seems more applicable to computational assignments, and this was partially shown in the reported results of numerical experiments on typical testing functions.

References

1. Branin, F. (1972), Widely convergent methods for finding multiple solutions of simultaneous nonlinear equations, *IBM Journal of Research Development* 16: 504–522.
2. Branin, F. and Hoo, S. (1972), A method for finding multiple extrema of a function of n variables, in: Lootsma, F. (ed.), *Numerical Methods of Nonlinear Optimization*, pp. 231–237, Academic Press, London.
3. Dixon, L.C.W. and Szegö, G.P. (eds) (1975), *Towards Global Optimization*, North-Holland, Amsterdam.
4. Dixon, L.C.W. and Szegö, G.P. (eds) (1978), *Towards Global Optimization 2*, North-Holland, Amsterdam.
5. Ge, R. and Qin, Y. (1987), A class of filled functions for finding global minimizers of a function of several variables, *Journal of Optimization Theory and Applications* 54: 241–252.
6. Ge, R. (1990), A filled function method for finding a global minimizer of a function of several variables, *Mathematical Programming* 46: 191–204.
7. Ge, R. (1990), The globally convexized filled functions for global optimization, *Applied Mathematics and Computation* 35: 131–158.

8. Liu, X. (1987), *Several New Optimization Methods and Their Application to Electrical Engineering*, M.Sc. thesis, Department of Electrical Engineering, Jiaotong University.
9. Liu, X. (1992), *Global Minimization and Stochastic Programming*, M. Math. thesis, Department of Combinatorics and Optimization, the University of Waterloo.
10. Horst, R. and Tuy, H. (1996), *Global Optimization (Deterministic Approaches)* (3rd edn.), Springer-Verlag, Berlin.
11. Pardalos, P. and Rosen, J. (1987), *Constrained Global Optimization: Algorithms and Applications*, Springer-Verlag, Berlin.
12. Rastrigin, L. (1974), *Systems of Extremal Control*, Nauka, Moscow.
13. Törn, A. and Žilinskas, A. (1989), *Global Optimization*, Springer-Verlag, Berlin.