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Test Functions with Variable Attraction Regions for Global Optimization Problems ⋆

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Abstract. Functions with local minima and size of their 'region of attraction' known *a priori*, are often needed for testing the performance of algorithms that solve global optimization problems. In this paper we investigate a technique for constructing test functions for global optimization problems for which we fix *a priori*: (i) the problem dimension, (ii) the number of local minima, (iii) the local minima points, (iv) the function values of the local minima. Further, the size of the region of attraction of each local minimum may be made large or small. The technique consists of first constructing a convex quadratic function and then systematically distorting selected parts of this function so as to introduce local minima.

Key words: Global Optimization, Test problems

1. Introduction

The global optimization problem may be expressed as :

$$\text{find } x^* \in D,\ D \subset \mathbf{R}^n \text{ such that } f(x^*) \leq f(x), \quad \forall x \in D \tag{1.1}$$

where $f : D \longrightarrow \mathbf{R}$ and D is a compact set in $\mathbf{R}^n$. It is well-known that (1.1) is very difficult to solve because both the global minimum may have a 'small attraction region' and there do not exist simple rules to establish whether or not a given point is a global minimum. Test problems are needed to evaluate the efficiency of algorithms proposed for solving (1.1). Many global optimization test problems exist in the literature (e.g. Dixon & Szegö, 1978; Schittkowski, 1980, 1987; Floudas & Pardalos, 1990). In addition, test problem generators have been developed for specific problem classes (e.g. Sung & Rosen, 1982; Kalantari & Rosen, 1986; Pardalos, 1987, 1991; Li & Pardalos 1992; Khoury & Pardalos, 1993; Moshirvaziri, 1994; Jacobsen, 1996). The main drawback of test problems may be that the local minima and their function values are not known exactly *a priori*. Moreover, we have no estimate on the size of the 'attraction region' of each local minimum. For this concept we may consider the definition by Betró (1991).

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Let D be a compact set in $\mathbf{R}^n$. *Assume that in D there is a finite number of local minima, say* $x_1^*, \ldots, x_m^*$. *Let P be a search algorithm which, starting from a point* $x \in D$ *leads to some point P(x) in D. Then define region of attraction of* x_i^*, $i = 1, \ldots, m$, *the set*

$$X_i^* \equiv \{x \in D : P(x) = x_i^*\},\ i = 1, \ldots, m.$$

As has been done in previous papers (Pardalos, 1987; Li & Pardalos, 1992), in the present paper we investigate a technique for constructing test functions for global optimization problems for which we fix *a priori*

(1) the problem dimension;
(2) the number of local minima;
(3) the local minima points;
(4) the function values at the local minima;

and for which the size of the 'region of attraction' of each local minimum may be made large or small. The technique consists of redefining a paraboloid Z given on D within subsets $S_i \subset D,\ i = 1, \ldots, m$, by cubic and quintic interpolations.

2. Test function by cubic polynomials

Roughly speaking, our technique for constructing test functions by cubic polynomial consists of defining a paraboloid Z within a fixed domain $D \subset \mathbf{R}^n$, then in redefining the equation representing Z within balls $S_i \subset D$, $i = 1, \ldots, m$, of radius ρ_i, such that the resulting function f is continuously differentiable and has a local minimum in S_i. For simplicity we develop our construction technique in the case of a unique ball S of radius ρ.

Let us consider the paraboloid Z in a fixed domain $D \subset \mathbf{R}^n$ of equation

$$Z: \quad g(x) = \|x - T\|^2 + t, \quad x \in D \tag{2.1}$$

where $T = (\bar{x}_1, \ldots, \bar{x}_n) \in D$ and $t \in \mathbf{R}$ are fixed. By $\|\cdot\|$ we denote here and throughout the paper the euclidian norm. Clearly $g(x)$ has its minimum at T with value t. Denote by $M \equiv (y_1, \ldots, y_n)$ any point chosen in the interior of D, with $M \neq T$; let η denote the least distance from M to the boundary of D, ρ any positive real with $\rho < \min(\eta, \|M - T\|)^\star$, and

$$S = \{x \in \mathbf{R}^n |\ \|x - M\| \leq \rho\}, \qquad B = \mathcal{F}S \equiv \text{the boundary of } S \tag{2.2}$$

Our aim is to redefine Z in the ball S. Let $x \equiv (x_1, \ldots, x_n)$ be any point in S and Q be given by

$$Q \equiv \left(\rho\frac{(x_1 - y_1)}{\|x - M\|} + y_1, \ldots, \rho\frac{(x_n - y_n)}{\|x - M\|} + y_n\right).$$

* The subsequent investigation could be carried out with $\rho < \|M - T\|$.

Clearly $Q \in B$. We determine the univariate cubic polynomial $C(\lambda)$ such that

$$C(0) = f \quad C'(0) = 0; \qquad C(\rho) = \phi \quad C'(\rho) = \gamma \tag{2.3}$$

where ϕ and γ are the values of Z at Q and the directional derivative of Z along the segment from Q to M, respectively. Further f is any arbitrary real such that $f \le \bar{f} = \min\{g(x)|x \in B\}$, that is

$$\begin{aligned}\phi &= \sum_{k=1}^{n}\left[\frac{\rho(x_k - y_k)}{\|x - M\|} + y_k - \bar{x}_k\right]^2 + t\\ \gamma &= 2\sum_{k=1}^{n}\left[\frac{\rho(x_k - y_k)}{\|x - M\|} + y_k - \bar{x}_k\right]\frac{x_k - y_k}{\|x - M\|}.\end{aligned} \tag{2.4}$$

Straightforward computations give

$$C(\lambda) = a\lambda^3 + b\lambda^2 + f \tag{2.5}$$

with

$$a = -\frac{2}{\rho^3}(\phi - f) + \frac{\gamma}{\rho^2}, \qquad b = -\frac{3}{\rho^2}(\phi - f) + \frac{\gamma}{\rho}.$$

At this point for any $x \equiv (x_1, \dots, x_n) \in S$ we define the function

$$\begin{aligned}C_\rho(x) = &\left(\frac{2}{\rho^2}\frac{\langle x - M, T - M\rangle}{\|x - M\|} - \frac{2}{\rho^3}A\right)\|x - M\|^3\\ &+ \left(1 - \frac{4}{\rho}\frac{\langle x - M, T - M\rangle}{\|x - M\|} + \frac{3}{\rho^2}A\right)\|x - M\|^2 + f\end{aligned} \tag{2.6}$$

where $A = \|T - M\|^2 + t - f$, and $<, >$ denotes the usual scalar product.

Finally we define for $x \in D$

$$f(x) = \begin{cases} C_\rho(x) & \text{if} \quad x \in S\\ g(x) & \text{if} \quad x \notin S.\end{cases} \tag{2.7}$$

We can show the following:

LEMMA 2.1. *$f(x)$ given by (2.7) is continuously differentiable in D.*

Proof. Consider the first order derivatives; we have for $x \in D$

$$\frac{\partial f(x)}{\partial x_j} = \begin{cases} \frac{\partial C_\rho(x)}{\partial x_j} & \text{if} \quad x \in S\\ 2(x_j - \bar{x}_j) & \text{if} \quad x \notin S\end{cases} \tag{2.8}$$

where

$$\begin{aligned}\frac{\partial C_\rho(x)}{\partial x_j} =& \frac{2}{\rho^2} h_j(x)\|x-M\| + 3\left(\frac{2}{\rho^2}\frac{\langle x-M, T-M\rangle}{\|x-M\|} - \frac{2}{\rho^3}A\right)\\ &\times (x_j - y_j)\|x-M\| - \frac{4}{\rho}h_j(x)\\ &+ 2\left(1 - \frac{4}{\rho}\frac{\langle x-M, T-M\rangle}{\|x-M\|} + \frac{3}{\rho^2}A\right)(x_j - y_j)\end{aligned}$$

with $h_j(x) = (\bar{x}_j - y_j)\|x-M\| - \langle x-M, T-M\rangle(x_j - y_j)/\|x-M\|$. That is

$$\begin{aligned}\frac{\partial C_\rho(x)}{\partial x_j} =& \frac{2}{\rho^2} h_j(x)\|x-M\| + \frac{6}{\rho^2}\langle x-M, T-M\rangle(x_j - y_j)\\ &- \frac{6}{\rho^3}A(x_j - y_j)\|x-M\| - \frac{4}{\rho}h_j(x) + 2(x_j - y_j)\\ &- \frac{8}{\rho}\frac{\langle x-M, T-M\rangle}{\|x-M\|}(x_j - y_j) + \frac{6}{\rho^2}A(x_j - y_j).\end{aligned}$$

We evaluate $\partial C_\rho/\partial x_j$ at any $x \in B$. Substituting $\|x-M\|$ for ρ into $\partial C_\rho/\partial x_j$ we get

$$\begin{aligned}&(2/\rho^2)\, h_j(x)\rho + (6/\rho^2)\langle x-M, T-M\rangle(x_j - y_j)\\ &\quad - (6/\rho^2)\, A(x_j - y_j) - (4/\rho)\, h_j(x) + 2(x_j - y_j)\\ &\quad - (8/\rho^2)\langle x-M, T-M\rangle(x_j - y_j) + (6/\rho^2)\, A(x_j - y_j)\\ &= -(2/\rho)\, h_j(x) - (2/\rho^2)\langle x-M, T-M\rangle(x_j - y_j) + 2(x_j - y_j)\\ &= -2(\bar{x}_j - y_j) + (2/\rho^2)\langle x-M, T-M\rangle(x_j - y_j)\\ &\quad - (2/\rho^2)\langle x-M, T-M\rangle(x_j - y_j) + 2(x_j - y_j)\\ &= 2(x_j - \bar{x}_j)\end{aligned}$$

Clearly continuity at $x \in B$ follows. To complete the proof we need to show the continuity of $\partial f/\partial x_j$ at M. We calculate $\lim_{x\to M} \partial f/\partial x_j$. In the expression for $\partial f/\partial x_j$ the only term whose limit is not trivial is

$$-\frac{4}{\rho}(x_j - y_j)\frac{\langle x-M, T-M\rangle}{\|x-M\|},$$

which may be written as

$$-\frac{4}{\rho}(x_j - y_j)\theta(x)\|T-M\|$$

with $|\theta(x)| < 1$. The latter goes to zero as $x \to M$. □

LEMMA 2.2. *The cubic polynomial $C(\lambda)$ has a minimum at $\lambda = 0$.*

Proof. The second order derivative of $C(\lambda)$ at zero equals:

$$\frac{d^2C}{d\lambda^2}(0) = 2b = 2\left[\frac{3}{\rho^2}(\phi - f) - \frac{\gamma}{\rho}\right]$$

with ϕ and γ defined in (2.4). It is not restrictive to assume $x \in B$. In this case

$$\phi = \sum_{k=1}^{n}(x_k - \bar{x}_k)^2 + t \qquad \gamma = 2\sum_{k=1}^{n}(x_k - \bar{x}_k)\frac{(x_k - y_k)}{\rho}$$

and

$$\begin{aligned} \rho^2 b &= \rho^2\left[\frac{3}{\rho^2}(\phi - f) - \frac{\gamma}{\rho}\right] \\ &=< x - T, (x - M) - 3(T - M) > +3(t - f) \\ &=< v_1, v_2 > +3(t - f) \end{aligned} \tag{2.9}$$

where $v_1 \equiv (x - T)$ and $v_2 \equiv (x - M) - 3(T - M) \equiv (x - 3T + 2M)$.

The scalar product $\langle v_1, v_2\rangle$ may be given as function of θ, with $\cos(\theta) = \langle x - M, T - M\rangle/(\|x - M\|\|T - M\|)$. Let

$$w = (T - M)/\|T - M\| = (w_1, \dots, w_n)$$

and

$$z = (x - x_p)/\|x - x_p\| = (z_1, \dots, z_n)$$

where x_p is the projection of x onto $(T - M)$. Then we may write

$$x \equiv (w_1\rho\cos\theta + z_1\rho\sin\theta + y_1, \dots, w_n\rho\cos\theta + z_n\rho\sin\theta + y_n).$$

Moreover,

$$\begin{aligned} v_1 &\equiv (x - T) \\ &\equiv (w_1\rho\cos\theta + z_1\rho\sin\theta + y_1 - \bar{x}_1, \dots, w_n\rho\cos\theta + z_n\rho\sin\theta + y_n - \bar{x}_n) \end{aligned}$$

and

$$\begin{aligned} v_2 &\equiv (x - 3T + 2M) \\ &\equiv (w_1\rho\cos\theta + z_1\rho\sin\theta + 3y_1 - 3\bar{x}_1, \dots, w_n\rho\cos\theta + z_n\rho\sin\theta \\ &\quad + 3y_n - 3\bar{x}_n). \end{aligned}$$

Since $\langle z, w\rangle = 0$ and $\langle z, T - M\rangle = 0$ we have

$$\begin{aligned}
&\langle v_1, v_2\rangle = \\
&\sum_{i=1}^{n}(w_i\rho\cos\theta + z_i\rho\sin\theta + y_i - \bar{x}_i)(w_i\rho\cos\theta + z_i\rho\sin\theta + 3y_i - 3\bar{x}_i) \\
&= \rho^2\cos^2\theta\|w\|^2 + \rho^2\sin^2\theta\|z\|^2 + 2\rho^2\sin\theta\cos\theta(w_1z_1 + \cdots + w_nz_n) \\
&\quad - 4\rho\cos\theta[(\bar{x}_1 - y_1)w_1 + \cdots + (\bar{x}_n - y_n)w_n] \\
&\quad - 4\rho\sin\theta[(\bar{x}_1 - y_1)z_1 + \cdots + (\bar{x}_n - y_n)z_n] - 6(\bar{x}_1y_1 + \cdots + \bar{x}_ny_n) \\
&= \rho^2 - 4\rho\cos\theta\|T - M\|\langle w, w\rangle - 6\sum_{i=1}^{n}\bar{x}_iy_i \\
&= \rho^2 - 4\rho\cos\theta\|T - M\| - 6\langle T, M\rangle.
\end{aligned}$$

Hence $\langle v_1, v_2\rangle$ has its minimum at $\theta = 0$, which implies x lying in the segment from M to T. This is true for b too. At this point we calculate $\rho^2 b$ at $\theta = 0$. We get

$$\rho^2 b = -\tau\rho + 3(\tau + \rho)\tau + 3(t - f)$$

with $\tau = \|x - T\|$.

Further since we assumed $f < \bar{f}$, with $\bar{f}$ being the minimum of the paraboloid (2.1) in the set B, that is $\bar{f} = \tau^2 + t$, we have

$$\rho^2 b = 3\tau^2 + 2\tau\rho + 3(t - \bar{f}) = 3\tau^2 + 2\tau\rho - 3\tau^2 = 2\tau\rho > 0.$$

This completes the proof. □

LEMMA 2.3. *M is the unique local minimum of $f(x)$ in S.*

Proof. First note that by definition $f(x)$ must have at least one local minimum in S. Assume the lemma is false. Then there exists a point $R \equiv (x) \in S$, $R \neq M$, that is a local minimum of $f(x)$ in S. Let $C(\lambda)$ be the cubic polynomial constructed according to (2.3) with ϕ and γ calculated with respect to R. Because of Lemma 2.2, and since Lemma 2.3 is assumed to be false, $C(\lambda)$ has two local minima. Clearly, this contradiction proves the lemma. □

3. Test function by quintic polynomials

In the preceding paragraph we constructed a continuously differentiable test function redefining the paraboloid Z by cubic polynomials. Now we generalize this procedure by using quintic polynomials such that the redefined function is twice continuously differentiable. Let M, T, S and B be defined as in Section 2. Proceeding much the same way as in Section 2, first we write the quintic polynomial

$Q(\lambda)$ such that

$$\begin{array}{lll} Q(0) = f & Q'(0) = 0 & Q''(0) = \delta \\ Q(\rho) = \phi & Q'(\rho) = \gamma & Q''(\rho) = 2 \end{array} \tag{3.1}$$

where ϕ and γ are defined in (2.4) and δ is an arbitrary positive real number. Note that the second directional derivative of Z at any point and along any direction is constant, that is 2. Further, f is any real number such that $f \leq \bar{f} = \min\{g(x) \| x \in B\}$. The equation of $Q(\lambda)$ satisfying $Q(0) = f,\ Q'(0) = 0$ is

$$Q(\lambda) = a\lambda^5 + b\lambda^4 + c\lambda^3 + d\lambda^2 + f \tag{3.2}$$

with a, b, c, d parameters to calculate. By taking into account the remaining conditions of (3.1) and solving with respect to a, b, c and d, we get

$$\begin{aligned} a &= \frac{6}{\rho^5}(\phi - f) - \frac{3}{\rho^4}\gamma - \frac{1}{2}\frac{\delta}{\rho^3} + \frac{1}{\rho^3} \\ b &= -\frac{15}{\rho^4}(\phi - f) + \frac{7}{\rho^3}\gamma + \frac{3}{2}\frac{\delta}{\rho^2} - \frac{2}{\rho^2} \\ c &= \frac{10}{\rho^3}(\phi - f) - \frac{4}{\rho^2}\gamma - \frac{3}{2}\frac{\delta}{\rho} + \frac{1}{\rho} \\ d &= \frac{1}{2}\delta. \end{aligned}$$

Since $\|x - M\| = \lambda$, and recalling ϕ and γ given in (2.4), we define the function $Q_\rho(x)$, for any $x \in S$.

$$\begin{aligned} Q_\rho(x) = & \left[-\frac{6}{\rho^4}\frac{\langle x - M, T - M\rangle}{\|x - M\|} + \frac{6}{\rho^5}A + \frac{1}{\rho^3}\left(1 - \frac{\delta}{2}\right)\right]\|x - M\|^5 \\ & + \left[\frac{16}{\rho^3}\frac{\langle x - M, T - M\rangle}{\|x - M\|} - \frac{15}{\rho^4}A - \frac{3}{\rho^2}\left(1 - \frac{\delta}{2}\right)\right]\|x - M\|^4 \\ & + \left[-\frac{12}{\rho^2}\frac{\langle x - M, T - M\rangle}{\|x - M\|} + \frac{10}{\rho^3}A + \frac{3}{\rho}\left(1 - \frac{\delta}{2}\right)\right]\|x - M\|^3 \\ & + \frac{1}{2}\delta\|x - M\|^2 + f \end{aligned} \tag{3.3}$$

with $A = \|T - M\|^2 + t - f$. Then the function defined for any $x \in D$ is

$$f(x) = \begin{cases} Q_\rho(x) & \text{if} \quad x \in S \\ g(x) & \text{if} \quad x \notin S. \end{cases} \tag{3.4}$$

We can prove

LEMMA 3.1. *$f(x)$ is twice continuously differentiable.*

Proof. The first order derivatives of $f(x)$ are

$$\frac{\partial f(x)}{\partial x_j} = \begin{cases} \frac{\partial Q_\rho(x)}{\partial x_j} & \text{if} \quad x \in S \\ 2(x_j - \bar{x}_j) & \text{if} \quad x \notin S \end{cases} \tag{3.5}$$

for $j = 1, \dots, n$ and

$$\begin{aligned} \frac{\partial Q_\rho(x)}{\partial x_j} = & - \frac{6}{\rho^4} h_j(x) \|x - M\|^3 \\ & + 5\left[-\frac{6}{\rho^4} \frac{\langle x - M, T - M \rangle}{\|x - M\|} + \frac{6}{\rho^5} A + \frac{1}{\rho^3}\left(1 - \frac{\delta}{2}\right)\right] \\ & \times (x_j - y_j)\|x - M\|^3 + \frac{16}{\rho^3} h_j(x)\|x - M\|^2 \\ & + 4\left[\frac{16}{\rho^3} \frac{\langle x - M, T - M \rangle}{\|x - M\|} - \frac{15}{\rho^4} A - \frac{3}{\rho^2}\left(1 - \frac{\delta}{2}\right)\right] \\ & \times (x_j - y_j)\|x - M\|^2 - \frac{12}{\rho^2} h_j(x)\|x - M\| \\ & + 3\left[-\frac{12}{\rho^2} \frac{\langle x - M, T - M \rangle}{\|x - M\|} + \frac{10}{\rho^3} A + \frac{3}{\rho}\left(1 - \frac{\delta}{2}\right)\right] \\ & \times (x_j - y_j)\|x - M\| + \delta(x_j - y_j) \end{aligned} \tag{3.6}$$

with $h_j(x) = (\bar{x}_j - y_j)\|x - M\| - \langle x - M, T - M \rangle (x_j - y_j)/\|x - M\|$.

We need to consider $\partial Q_\rho(x)/\partial x_j$ in the set B, that is for x such that $\|x - M\| = \rho$. We obtain

$$\begin{aligned} & - (2/\rho)\, h_j(x) - (2/\rho^2)\, \langle x - M, T - M \rangle (x_j - y_j) \\ & + 2(x_j - y_j)(1 - \delta/2) + \delta(x_j - y_j) \\ = & - 2(\bar{x}_j - y_j) + (2/\rho^2)\, \langle x - M, T - M \rangle (x_j - y_j) \\ & - (2/\rho^2)\, \langle x - M, T - M \rangle (x_j - y_j) + 2(x_j - y_j) \\ = & 2(x_j - \bar{x}_j). \end{aligned}$$

Since

$$\lim_{P \to M} \frac{\partial Q_\rho(x)}{\partial x_j} = 0, \quad \text{for} \;\; j = 1, \dots, n$$

it follows that $f(x)$ is continuously differentiable. Now we consider the second order derivatives $\partial^2 f(x)/\partial x_j \partial x_k$ and $\partial^2 f(x)/\partial x_j^2$. We have for $j, k = 1, \dots, n,\; j \neq k$

$$\frac{\partial^2 f(x)}{\partial x_j \partial x_k} = \begin{cases} \frac{\partial^2 Q_\rho(x)}{\partial x_j \partial x_k} & \text{if} \quad x \in S \\ 0 & \text{if} \quad x \notin S \end{cases}$$

where

$$
\begin{aligned}
\frac{\partial^2 Q_\rho(x)}{\partial x_j \partial x_k} = & -\frac{6}{\rho^4}\left[\frac{\partial h_j(x)}{\partial x_k}\|x-M\|^3 + 3h_j(x)(x_k-y_k)\|x-M\|\right] \\
& -\frac{30}{\rho^4}h_k(x)(x_j-y_j)\|x-M\| \\
& +15\left[-\frac{6}{\rho^4}\frac{\langle x-M, T-M\rangle}{\|x-M\|} + \frac{6}{\rho^5}A + \frac{1}{\rho^3}\left(1-\frac{\delta}{2}\right)\right] \\
& \times (x_j-y_j)(x_k-y_k)\|x-M\| \\
& +\frac{16}{\rho^3}\left[\frac{\partial h_j(x)}{\partial x_k}\|x-M\|^2 + 2h_j(x)(x_k-y_k)\right] \\
& +\frac{64}{\rho^3}h_k(x)(x_j-y_j) \\
& +8\left[\frac{16}{\rho^3}\frac{\langle x-M, T-M\rangle}{\|x-M\|} - \frac{15}{\rho^4}A - \frac{3}{\rho^2}\right. \\
& \times \left.\left(1-\frac{\delta}{2}\right)\right](x_j-y_j)(x_k-y_k) \\
& -\frac{12}{\rho^2}\left[\frac{\partial h_j(x)}{\partial x_k}\|x-M\| + h_j(x)\frac{(x_k-y_k)}{\|x-M\|}\right] \\
& -\frac{36}{\rho^2}h_k(x)\frac{(x_j-y_j)}{\|x-M\|} \\
& +3\left[-\frac{12}{\rho^2}\frac{\langle x-M, T-M\rangle}{\|x-M\|} + \frac{10}{\rho^3}A + \frac{3}{\rho}\left(1-\frac{\delta}{2}\right)\right] \\
& \times (x_j-y_j)\frac{(x_k-y_k)}{\|x-M\|},
\end{aligned}
$$

with

$$
\frac{\partial h_j(x)}{\partial x_k} = (\bar{x}_j - y_j)\frac{(x_k-y_k)}{\|x-M\|} - \frac{h_k(x)}{\|x-M\|^2}(x_j-y_j)
$$

$$
h_k(x) = (\bar{x}_k - y_k)\|x-M\| - \langle x-M, T-M\rangle\frac{(x_k-y_k)}{\|x-M\|}
$$

and for $j = 1, \dots, n$

$$
\frac{\partial^2 f(x)}{\partial x_j^2} = \begin{cases} \frac{\partial^2 Q_\rho(x)}{\partial x_j^2} & \text{if} \quad x \in S \\ 2 & \text{if} \quad x \notin S \end{cases}
$$

where

$$
\begin{aligned}
\frac{\partial^2 Q_\rho(x)}{\partial x_j^2} =&-\frac{6}{\rho^4}\left[\frac{\partial h_j(x)}{\partial x_j}\|x-M\|^3+3h_j(x)(x_j-y_j)\|x-M\|\right]\\
&-\frac{30}{\rho^4}h_j(x)(x_j-y_j)\|x-M\|\\
&+\left[-\frac{6}{\rho^4}\frac{\langle x-M,T-M\rangle}{\|x-M\|}+\frac{6}{\rho^5}A+\frac{1}{\rho^3}\left(1-\frac{\delta}{2}\right)\right]\\
&\times\left[5\|x-M\|^3+15(x_j-y_j)^2\|x-M\|\right]\\
&+\frac{16}{\rho^3}\left[\frac{\partial h_j(x)}{\partial x_j}\|x-M\|^2+2h_j(x)(x_j-y_j)\right]\\
&+\frac{64}{\rho^3}h_j(x)(x_j-y_j)\\
&+\left[\frac{16}{\rho^3}\frac{\langle x-M,T-M\rangle}{\|x-M\|}-\frac{15}{\rho^4}A-\frac{3}{\rho^2}\left(1-\frac{\delta}{2}\right)\right]\\
&\times\left[4\|x-M\|^2+8(x_j-y_j)^2\right]\\
&-\frac{12}{\rho^2}\left[\frac{\partial h_j(x)}{\partial x_j}\|x-M\|+h_j(x)\frac{(x_j-y_j)}{\|x-M\|}\right]\\
&-\frac{36}{\rho^2}h_j(x)\frac{(x_j-y_j)}{\|x-M\|}\\
&+\left[-\frac{12}{\rho^2}\frac{\langle x-M,T-M\rangle}{\|x-M\|}+\frac{10}{\rho^3}A+\frac{3}{\rho}\left(1-\frac{\delta}{2}\right)\right]\\
&\times\left[\|x-M\|+3\frac{(x_j-y_j)^2}{\|x-M\|}\right]+\delta
\end{aligned}
$$

with

$$\frac{\partial h_j(x)}{\partial x_j}=(\bar{x}_j-y_j)\frac{(x_j-y_j)}{\|x-M\|}-\frac{h_j(x)}{\|x-M\|^2}(x_j-y_j)-\frac{\langle x-M,T-M\rangle}{\|x-M\|}.$$

We need to investigate $\partial^2 Q_\rho/(\partial x_j\partial x_k)$, $j,k=1,\dots,n$, in the set B. Substituting $\|x-M\|=\rho$ in these derivatives, straigthforward computations give

$$\left(\frac{\partial^2 Q_\rho}{\partial x_j\partial x_k}\right)_B=0 \qquad \left(\frac{\partial^2 Q_\rho}{\partial x_j^2}\right)_B=2 \qquad j,k=1,\dots,n; \quad j\neq k$$

and the continuity of $\partial^2 f/(\partial x_j\partial x_k)$, $(j,k=1,\dots,n)$ in B follows. We conclude the proof by verifying the continuity of the second derivatives of $f(x)$ at M. Since

$$\left|\frac{\langle x-M,T-M\rangle}{\|x-M\|}\right|<\|T-M\| \tag{3.7}$$

and

$$\frac{x_j - y_j}{\|x - M\|} < 1 \tag{3.8}$$

we get

$$\lim_{x\to M} h_j(x) = 0. \tag{3.9}$$

At this point, it is easy to show that (3.7), (3.8) and (3.9) imply

$$\lim_{x\to M} \frac{\partial^2 f(x)}{\partial x_j \partial x_k} = 0, \quad j \neq k.$$

Proceeding much the same way we get

$$\lim_{x\to M} \frac{\partial^2 f(x)}{\partial x_j^2} = \delta \qquad \square$$

We now want to show that a lemma similar to Lemma 2.3 holds for $f(x)$ defined by (3.4). We need to prove the following lemma first.

LEMMA 3.2. *Let* $\lambda \in (0, \rho)$ *be fixed,* $G = \{x \in \mathbf{R}^n \,|\, \|x - M\| = \lambda\}$*, and* $P_1, \ P_2 \in G$. *If* $\theta_2 < \theta_1$ *with*

$$\cos\theta_i = \frac{\langle P_i - M, T - M\rangle}{\|P_i - M\|\|T - M\|}, \quad i = 1, 2$$

then $f(P_2) < f(P_1)$.

Proof. Let $P \in S, \ P \equiv (x)$; we can write

$$\begin{aligned}\phi(\theta) = & f(x_1, \ldots, x_n) = \left[\frac{1}{\rho^3}\left(1 - \frac{\delta}{2}\right) + \frac{6}{\rho^5}A - \frac{6}{\rho^4}\|T - M\|\cos\theta\right]\lambda^5 \\ & + \left[-\frac{3}{\rho^2}\left(1 - \frac{\delta}{2}\right) - \frac{15}{\rho^4}A + \frac{16}{\rho^3}\|T - M\|\cos\theta\right]\lambda^4 \\ & + \left[\frac{3}{\rho}\left(1 - \frac{\delta}{2}\right) + \frac{10}{\rho^3}A - \frac{12}{\rho^2}\|T - M\|\cos\theta\right]\lambda^3 \\ & + \frac{1}{2}\delta\lambda^2 + f \end{aligned} \tag{3.10}$$

with $A = \|M - T\|^2 + t - f$, $\lambda = \|P - M\|$ and $\theta \in [0, \pi]$.

We rewrite (3.10) as

$$\begin{aligned}\phi(\theta) = & \left[\frac{1}{\rho^3}\left(1 - \frac{\delta}{2}\right) + \frac{6}{\rho^5}A\right]\lambda^5 + \left[-\frac{3}{\rho^2}\left(1 - \frac{\delta}{2}\right) - \frac{15}{\rho^4}A\right]\lambda^4 \\ & + \left[\frac{3}{\rho}\left(1 - \frac{\delta}{2}\right) + \frac{10}{\rho^3}A\right]\lambda^3 + \frac{1}{2}\delta\lambda^2 + f \\ & + \|T - M\|\cos\theta\left[-\frac{6}{\rho^4}\lambda^2 + \frac{16}{\rho^3}\lambda - \frac{12}{\rho^2}\right]\lambda^3 \end{aligned}$$

Since

$$\left[-\frac{6}{\rho^4}\lambda^2+\frac{16}{\rho^3}\lambda-\frac{12}{\rho^2}\right]<0 \quad \forall\lambda\in(0,\rho)$$

and $\cos\theta$ decreases in $[0,\pi]$, the lemma is proved. □

LEMMA 3.3. *M is the unique local minimum of $f(x)$, $f(x)$ defined by (3.4), in the set S.*

Proof. First note that by definition $f(x)$ must have at least one local minimum in S. Assume there is a local minimum $M^*\neq M$, $M^*\in S$. Let

$$\cos\theta^*=\frac{\langle M^*-M,T-M\rangle}{\|M^*-M\|\|T-M\|};$$

θ^* cannot be zero. Indeed, in this case the quintic polynomial through M and M^* defined in (3.2) would have first and second order derivatives at $\lambda=\rho$ negative while the directional derivatives γ and δ are negative and positive, respectively. $\theta^*\neq 0$ and M being a local minimum imply the existence of $P\in S$ such that

$$\|P-M\|=\lambda^*, \qquad \lambda^*=\|M^*-M\|$$

$$\theta^*<\bar\theta, \qquad f(P)>f(M^*)$$

with

$$\cos\bar\theta=\frac{\langle P-M,T-M\rangle}{\|P-M\|\|T-M\|}$$

Clearly we get a contradiction with respect to Lemma 3.2. □

4. Test function construction

In this section we use the results of Sections 2 and 3 to define a test function $f(x)$ more general than that given by (2.7) or (3.4), and that exhibits the desiderable features listed in the introduction. For simplicity we assume that the domain D where the global minimum is sought is an interval in $\mathbf{R}^n$, that is

$$D=\{x\in\mathbf{R}^n\,|\,l_j\leq x_j\leq u_j,\ j=1,\ldots,n\} \tag{4.1}$$

with $l\equiv(l_j),\ u\equiv(u_j),\ l,\ u\in\mathbf{R}^n$.

The test function $f(x)$ will have $m+1$ local minima: the point T, given in (2.1), and the points $M_i,\ i=1,\ldots,m,\ M_i\neq T,\ M_i\neq M_j$ with $i\neq j$. Further, $f(x)$ is constructed by redefining the paraboloid Z given in (2.1), within the sets S_i given by

$$S_i=\{x\in\mathbf{R}^n\,|\,\|x-M_i\|\leq\rho_i\} \quad i=1,\ldots,m. \tag{4.2}$$

The choice of ρ_i is done under the following two constraints: (i) the sets S_i do not overlap; (ii) each S_i is entirely contained in D. These conditions are satisfied by requiring for $i = 1, \ldots, m$

$$\rho_i \leq \min(\text{bound}_i, \text{dist}_i)$$

with

$$\text{bound}_i = \min_j \left(u_j - y_{ij}, y_{ij} - l_j\right)$$

$$\text{dist}_i = \min\left(\min_{k \neq i} \|M_i - M_k\|, \|M_i - T\|\right) \tag{4.3}$$

with $M_i \equiv (y_{i1}, \ldots, y_{in})$.

Hence the ρ_i are chosen according to

$$\rho_i = w_i \ \min(\text{bound}_i, \text{dist}_i). \tag{4.4}$$

where $w_i \in (0, 1)$. The w_i are scaling factors in the interval $(0, 1)$; they may be used to increase or decrease ρ_i. Finally, our test function, in the case of cubic interpolation, is defined by

$$f(x) = \begin{cases} C_k(x) & \text{if} \quad x \in S_k,\ k \in \{1, \ldots, m\} \\ \|x - T\|^2 + t & \text{if} \quad x \notin S_1 \cup \cdots \cup S_m. \end{cases}$$

where

$$C_k(x) = \left(\frac{2}{\rho_k^2} \frac{\langle x - M_k, T - M_k \rangle}{\|x - M_k\|} - \frac{2}{\rho_k^3} A\right) \|x - M_k\|^3$$
$$+ \left(1 - \frac{4}{\rho_k} \frac{\langle x - M_k, T - M_k \rangle}{\|x - M_k\|} + \frac{3}{\rho_k^2} A\right) \|x - M_k\|^2 + f_k$$

with $A = \|T - M_k\|^2 + t - f_k$ and $f_i \in \mathbf{R}$ such that

$$f_i \leq \min\{g(x) | x \in B_i\}, \qquad B_i = \{x \in \mathbf{R}^n | \ \|x - M_i\| = \rho_i\} \tag{4.5}$$

The test function based on the quintic interpolation is defined by

$$f(x) = \begin{cases} Q_k(x) & \text{if} \quad x \in S_k,\ k \in \{1, \ldots, m\} \\ \|x - T\|^2 + t & \text{if} \quad x \notin S_1 \cup \cdots \cup S_m. \end{cases}$$

where

$$Q_k(x) = \left[-\frac{6}{\rho_k^4} \frac{\langle x - M_k, T - M_k \rangle}{\|x - M_k\|} + \frac{6}{\rho_k^5} A + \frac{1}{\rho_k^3} \left(1 - \frac{\delta}{2}\right)\right] \|x - M_k\|^5$$
$$+ \left[\frac{16}{\rho_k^3} \frac{\langle x - M_k, T - M_k \rangle}{\|x - M_k\|} - \frac{15}{\rho_k^4} A - \frac{3}{\rho_k^2} \left(1 - \frac{\delta}{2}\right)\right] \|x - M_k\|^4$$
$$+ \left[-\frac{12}{\rho_k^2} \frac{\langle x - M_k, T - M_k \rangle}{\|x - M_k\|} + \frac{10}{\rho_k^3} A + \frac{3}{\rho_k} \left(1 - \frac{\delta}{2}\right)\right] \|x - M_k\|^3$$
$$+ \frac{1}{2} \delta \|x - M_k\|^2 + f_k$$

with $f_i \in \mathbf{R}$ satisfies (4.5).

To summarize, the following are the parameters to be assigned to define a test function.

(1) $l,\ u \in \mathbf{R}^n$ such that $l < u$
(2) $T = (\bar{x}_1, \dots, \bar{x}_n),\ l_j < \bar{x}_j < u_j$
(3) m, the number of new local minima
(4) M_i in the interior of D, $i = 1, \dots, m$
(5) $w_i \in (0, 1),\ i = 1, \dots, m$
(6) $f_i \in \mathbf{R}$ such that $f_i \le \min\{g(x) | x \in B_i\},\ B_i = \{x \in \mathbf{R}^n | \|x - M_i\| = \rho_i\}$ and ρ_i is calculated by (4.4).

In Figures 1 and 2 the level sets of two functions *Cubfun1* and *Cubfun2*, respectively, constructed by using cubic interpolation, are shown. The following parameters have been chosen for both functions:

$$l_i = -1, \quad u_i = 1, \quad i = 1, 2; \quad T \equiv (0, 0).$$

In particular, for *Cubfun1* we have

No. local minima $m = 3$

$M_1 = (-0.2135,\ -0.7038)$	$f_1 = 1.900$	$\rho_1 = 0.2962$
$M_2 = (-0.5621,\ 0.3586)$	$f_2 = 1.525$	$\rho_2 = 0.3334$
$M_3 = (0.3577,\ -0.2330)$	$f_3 = 1.200$	$\rho_3 = 0.2134$

For *Cubfun2* we have

No. local minima $m = 8$

$M_1 = (0.8694,\ -0.9146)$	$f_1 = 2.2000$	$\rho_1 = 0.0854$
$M_2 = (0.0388,\ -0.8663)$	$f_2 = 2.0000$	$\rho_2 = 0.1337$
$M_3 = (-0.2330,\ -0.2332)$	$f_3 = 1.8503$	$\rho_3 = 0.1648$
$M_4 = (-0.6734,\ 0.3998)$	$f_4 = 1.7286$	$\rho_4 = 0.2835$
$M_5 = (-0.1252,\ 0.2550)$	$f_5 = 1.4571$	$\rho_5 = 0.1420$
$M_6 = (0.3586,\ 0.3423)$	$f_6 = 1.1857$	$\rho_6 = 0.1543$
$M_7 = (0.2997,\ 0.0394)$	$f_7 = 0.9143$	$\rho_7 = 0.1511$
$M_8 = (0.6619,\ -0.1650)$	$f_8 = 0.5000$	$\rho_8 = 0.2079$

In Figures 3 and 4 the level sets of two functions *Quinfun1* and *Quinfun2*, constructed by using quintic interpolation, are shown.

The following parameters have been chosen for both functions:

$$l_i = -1, \quad u_i = 1, \quad i = 1, 2; \quad T \equiv (0, 0).$$

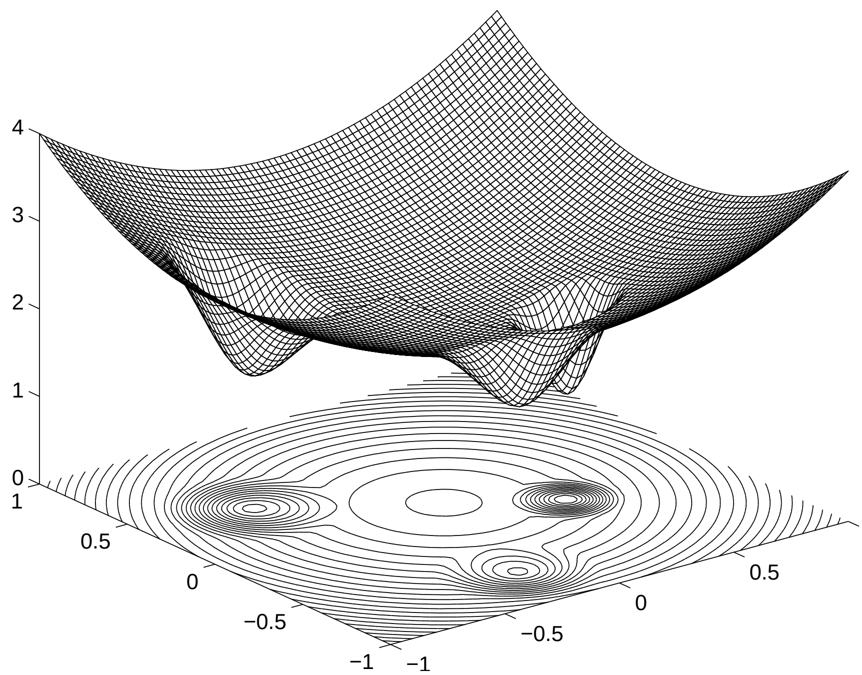

Figure 1. Graph of *Cubfun1*

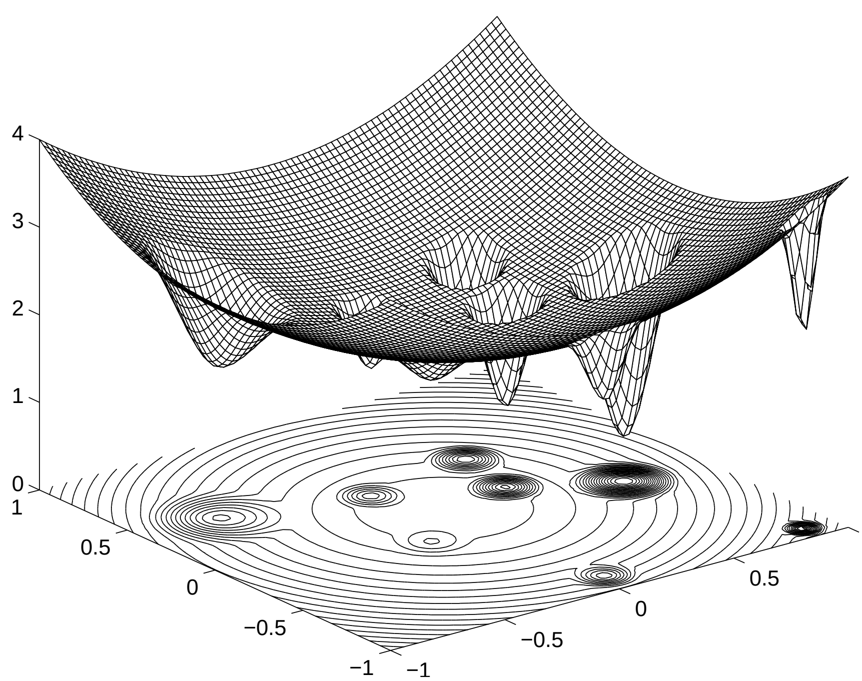

Figure 2. Graph of *Cubfun2*

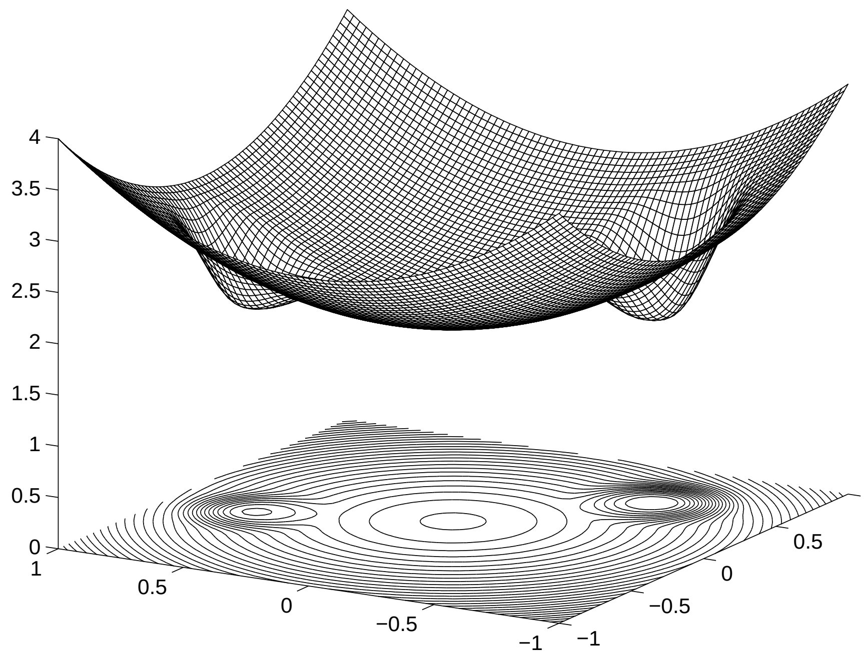

Figure 3. Graph of *Quinfun1*

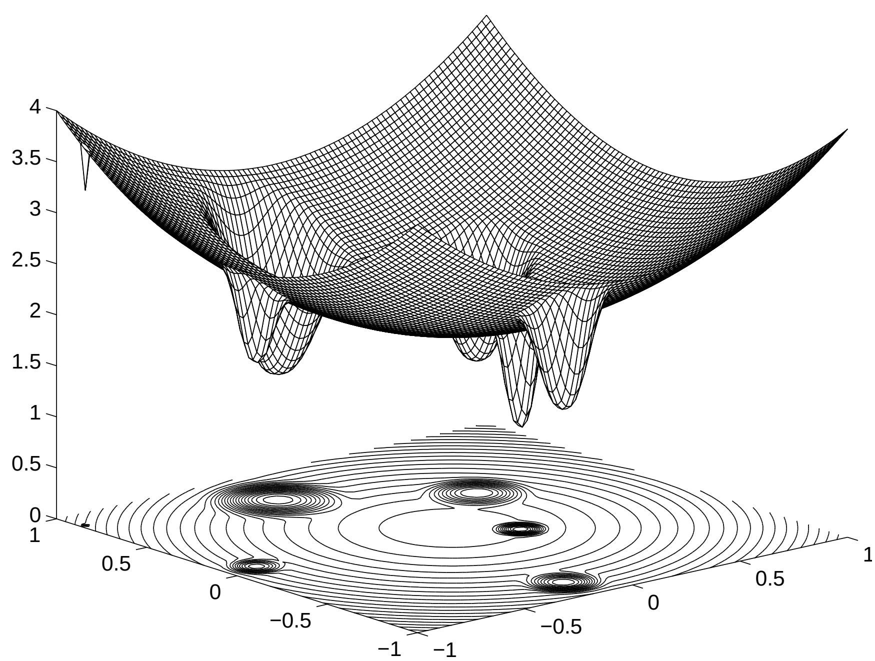

Figure 4. Graph of *Quinfun2*

Specifically for *Quinfun1* we have

$$\text{No. local minima } m = 2$$

$M_1 = (-0.2330,\ 0.6619)$	$f_1 = 2.0000$	$\rho_1 = 0.3381$
$M_2 = (0.5673,\ -0.4863)$	$f_2 = 1.8000$	$\rho_2 = 0.3727$

For *Quinfun2* we have

$$\text{No. local minima } m = 6$$

$M_1 = (-0.9846,\ 0.8609)$	$f_1 = 2.5000$	$\rho_1 = 0.0154$
$M_2 = (-0.8663,\ 0.0539)$	$f_2 = 2.0000$	$\rho_2 = 0.1337$
$M_3 = (-0.1650,\ -0.8161)$	$f_3 = 1.7000$	$\rho_3 = 0.1839$
$M_4 = (0.3735,\ 0.3078)$	$f_4 = 1.3000$	$\rho_4 = 0.2420$
$M_5 = (-0.2332,\ 0.6923)$	$f_5 = 1.2400$	$\rho_5 = 0.3077$
$M_6 = (0.1780,\ -0.1680)$	$f_6 = 1.0000$	$\rho_6 = 0.1224$

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