Journal of Global Optimization **25:** 175–181, 2003.

Rational Functions with Prescribed Global and Local Minimizers

ARNOLD NEUMAIER
Institut für Mathematik, Universität Wien, Strudlhofgasse 4, A-1090 Wien, Austria
(e-mail: arnold.neumaier@univie.ac.at; www: http://www.mat.univie.ac.at/∼neum/)

Abstract. A family of multivariate rational functions is constructed. It has strong local minimizers with prescribed function values at prescribed positions. While there might be additional local minima, such minima cannot be global. A second family of multivariate rational functions is given, having prescribed global minimizers and prescribed interpolating data.

Key words: Global optimization, test problems, prescribed global minimizers

1. Introduction

Testing global optimization algorithms is a nontrivial task, since many of the well-known test functions (for example, those in the classical test set by Dixon and Szegö [4]) are nowadays quite simplistic, and the global minima of more difficult functions are often not known.

Therefore it is desirable to have test functions that attain their global minimum at one or more predefined points, and that can be adjusted to match various difficulties, such as the existence of many local minimizers, ill-conditioned Hessian matrices at the optimizers (resulting in curved, narrow valleys), local minima close to a global one, narrow and deep holes, etc.

In this note, it is shown that this can be indeed achieved by two simple classes of rational functions in arbitrary dimensions.

In the following, $\|\cdot\| = \sqrt{x^T x}$ denotes the Euclidean norm of a vector x.

2. Prescribed global and local minimizers

THEOREM 2.1. *Let $x_1, \ldots, x_m \in \mathbb{R}^n$ be distinct, let $f_1, \ldots, f_m \in \mathbb{R}$, and let $R_1, \ldots, R_n \in \mathbb{R}^{n\times n}$ be triangular matrices with positive diagonal entries. Then the* *function*

$$f(x) = \begin{cases} f_k & \text{if } x = x_k \text{ for some } k, \\ \dfrac{\sum_k (2f_k + r_k(x))/r_k(x)^2}{\sum_k 2/r_k(x)^2} & \text{otherwise}, \end{cases} \tag{1}$$

where

$$r_k(x) = \|R_k(x - x_k)\|^2 \tag{2}$$

is infinitely often differentiable, and has strong local minimizers at $x = x_k$, with function values $f(x_k) = f_k$ and Hessian matrices $f''(x_k) = R_k^T R_k$. Moreover, the global minimizers of f are precisely the points x_k with $f_k = \min\{f_1, \ldots, f_m\}$.

Proof. In a sufficiently small neighbourhood of x_k we have

$$r_k(x_k + s) = \|R_k s\|^2 = s^T R_k^T R_k s = O(\|s\|^2).$$

Therefore

$$\begin{aligned} f(x_k + s) &= \Big(\frac{2f_k + r_k}{r_k^2} + O(1)\Big)\Big/\Big(\frac{2}{r_k^2} + O(1)\Big) \\ &= (2f_k + r_k + O(\|s\|^4))/(2 + O(\|s\|^4)), \end{aligned}$$

giving

$$f(x_k + s) = f_k + \frac{1}{2} s^T R_k^T R_k s + O(\|s\|^4). \tag{3}$$

This implies that

$$\lim_{s \to 0} f(x_k + s) = f_k,$$

providing continuity of f. Since f is rational for $x \notin \{x_1, \ldots, x_m\}$ and the denominators vanish only on this set, we see that f has no real poles and is therefore infinitely often differentiable. Comparison of (3) with the Taylor expansion shows that $f'(x_k) = 0$ and $f''(x_k) = R_k^T R_k$ is positive definite (since R_k is nonsingular). Therefore x_k is a strong local minimizer of f.

Now let $f_0 = \min_k f_k$. Then, for $x \notin \{x_1, \ldots, x_m\}$,

$$f(x) - f_0 = \frac{\sum_k (2(f_k - f_0) + r_k)/r_k^2}{\sum_k 2/r_k^2} > 0.$$

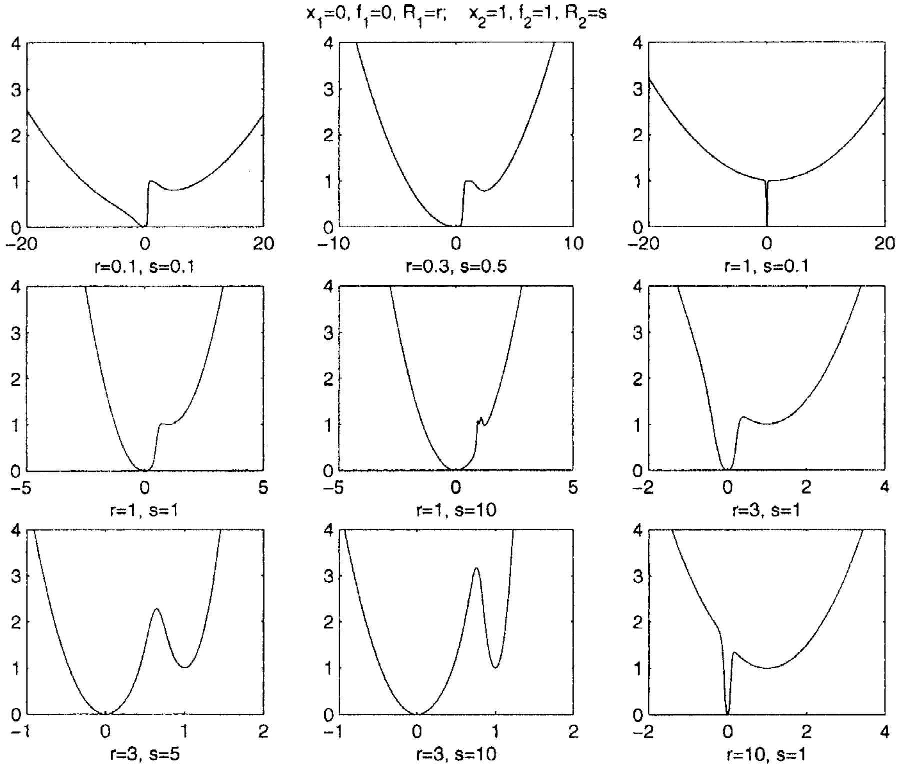

Figure 1. Rational functions with designed minima at $(x, f) = (0, 0)$ and $(1, 1)$.

On the other hand,

$$\min_k f(x_k) = \min_k f_k = f_0.$$

Therefore the global minimizers of f are precisely the x_k with $f_k = f_0$. □

EXAMPLE 2.2. To illustrate the flexibility of the construction we show in Figure 1 some univariate rational functions created with $x_1 = 0$, $f_1 = 0$, $x_2 = 1$, $f_2 = 1$ and various values for $r = R_1$ and $s = R_2$. We see (first two graphs) that there may be additional, undesigned local minima, and that sometimes a nonglobal designed minimum is hardly visible since it is only a small dip in a larger peak. As predicted by the theorem, the global minimizer is always at $x = 0$.

REMARKS 2.3.

(i) f may have additional local minimizers but, by the theorem, these cannot be global.

(ii) Far away from all points, $f(x)$ grows like $\|x\|^2$ in the sense that $f(x)/\|x\|^2$ remains bounded.

(iii) An arbitrary positive definite Hessian matrix G can be written in the form $G = R^T R$ with a triangular matrix with positive diagonal entries. This is achieved by means of a Cholesky factorization. Therefore the theory allows to prescribe the full quadratic Taylor approximation of arbitrary local minimizers.

(iv) For use as a test problem generator, we suggest that the function values f_k and the triangular matrices R_k are generated randomly. To get multiple global minima one simply replaces the smallest few f_k by $f_0 = \min_k f_k$. To get deep and narrow holes, multiply the corresponding R_k by a moderately large number. To get curved, narrow valleys, replace some diagonal entries of R_k by moderately small numbers. The positions of the local minimizers may be placed according to geometric patterns, or randomly. One can also place some minimizers much closer than the others. For test problems reported in publications, it is better to use $x_k,\ f_k,\ R_k$ rounded to simple values that can be explicitly given in a table (or in a file retrievable from the WWW).

In the most useful special case $m = 2$, the function (1) takes the form

$$f(x) = \frac{r_2(x)^2(2f_1 + r_1(x)) + r_1(x)^2(2f_2 + r_2(x))}{2(r_1(x)^2 + r_2(x)^2)}. \tag{4}$$

For example, for $f_1 = f_2 = 0, x_1 = u, x_2 = v \neq u, R_1 = R_2 = I$, (4) reduces to

$$f(x) = \frac{\|x-u\|^2\|x-v\|^2(\|x-u\|^2 + \|x-v\|^2)}{2(\|x-u\|^4 + \|x-v\|^4)}. \tag{5}$$

This function is always nonnegative, has precisely two global minimizers at $x = u$ and $x = v$, and satisfies

$$\frac{1}{2}\min(\|x-u\|^2, \|x-v\|^2) \leqslant f(x) \leqslant \frac{1}{2}\max(\|x-u\|^2, \|x-v\|^2).$$

A similar, somewhat simpler function with the same properties is

$$f(x) = \frac{\|x-u\|^2\ \|x-v\|^2}{2(\|x-u\|^2 + \|x-v\|^2)}. \tag{6}$$

3. Prescribed global minimizers and interpolation data

Törn and Zilinskas [11] proved that any method based on local information only that converges for every continuous f to a global minimizer of f in a feasible domain C must produce a sequence of points $x^1, x^2, \ldots$ that is dense in C. In particular, global optimization with function values only is an intrinsically ill-posed problem since without global information it is easy to miss minimizers lying in deep and narrow holes.

The following construction makes this explicit and provides further test problems, interpolating given data at a finite set of points but with arbitrarily positioned global minimizers.

THEOREM 3.1. *Given N pairs $(x_1, f_1), \ldots, (x_N, f_N) \in \mathbb{R}^n \times \mathbb{R}$, m points $\hat{x}_1, \ldots, \hat{x}_m \in \mathbb{R}^n$, a number $\hat{f} \in \mathbb{R}$ with $\hat{f} < \min_j f_j$, and m triangular matrices $R_1, \ldots, R_n \in \mathbb{R}^{n\times n}$ with positive diagonal entries, let*

$$f(x) = \hat{f} + p(x)^2 q(x), \tag{7}$$

$$q(x) = \frac{\prod_{k=1}^{m} \|R_k(x - \hat{x}_k)\|^2}{2(1 + \|B(x)\|^2)}$$

with arbitrary $B(x)$, and $p(x)$ is a function interpolating the following data:

$$p(\hat{x}_k) = \pm\sqrt{\frac{1 + \|B(\hat{x}_k)\|^2}{\prod_{l\neq k} \|R_l(\hat{x}_k - \hat{x}_l)\|^2}} \quad (k = 1, \ldots, m)$$

$$p(x_j) = \pm\sqrt{\frac{f_j - \hat{f}}{q(x_j)}} \quad (j = 1, \ldots, N)$$

Then f interpolates the given data,

$$f(x_j) = f_j \quad (j = 1 \ldots, N),$$

and has the global minimizers $\hat{x}_k (k = 1, \ldots, m)$ with global minimum value $\hat{f}$ and Hessians $f''(\hat{x}_k) = R_k^T R_k$.

Proof. The interpolation condition follows from $f(x_j) = \hat{f} + p(x_j)^2 q(x_j) = f_j$. Since $q(x) \geqslant 0$ with equality iff $x = \hat{x}_k$ for some k, (7) implies that $f(x)$ has global minimizers (at least) at the $\hat{x}_k$. To calculate the Hessians at these points, we note that the form of $q(x)$ implies that $q(\hat{x}_k) = 0$, $q'(\hat{x}_k) = 0$, and

$$q''(\hat{x}_k) = \frac{\prod_{l\neq k} \|R_l(\hat{x}_k - \hat{x}_l)\|^2}{1 + \|B(\hat{x}_k)\|^2} R_k^T R_k$$

since all other contributions to $q''(x)$ vanish at $x = \hat{x}_k$. Since all terms contributing to the Hessian f'' except $p^2 q''$ contain a factor q or q', we have

$$f''(\hat{x}_k) = p(\hat{x}_k)^2 q''(\hat{x}_k) = R_k^T R_k.$$

□

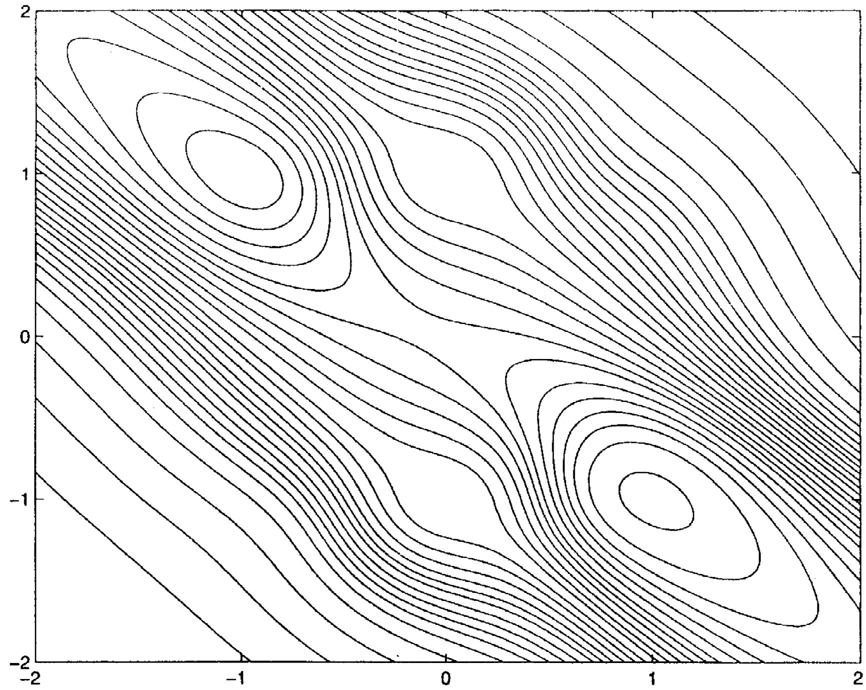

Figure 2. A rational function with designed global minima at $\binom{0}{1}$ and $\binom{0}{-1}$, and given values at $\binom{\pm 1}{\pm 1}$.

The theorem again illustrates the importance of global information, such as Lipschitz constants (e.g., Pinter [8]), curvature bounds (e.g., Brent [2]), interval extensions (e.g., Kearfott [5], Neumaier [6]) or explicit access to the analytical structure (Ryoo and Sahinidis [9], Neumaier et al. [7], Adjiman et al. [1]) for *reliable* global optimization.

EXAMPLE 3.2. We use $B(x) = 0$, and take $p(x)$ as the arbitrarily often differentiable Shepard interpolation function (Shepard [10])

$$p(x) = \begin{cases} p(z_l) & \text{if } x = z_l \text{ for some } l, \\ \sum_{l=1}^{m+N} p(z_l)\|x - z_l\|^{-2} \Big/ \sum_{l=1}^{m+N} \|x - z_l\|^{-2} & \text{otherwise}, \end{cases}$$

where $z_l = \hat{x}_l$ for $l \leqslant m$ and $z_l = x_{l-m}$ for $l > m$. Figure 2 contains level sets of a 2-dimensional example with $R_1 = R_2 = I$, interpolation points $\binom{1}{1}, \binom{1}{-1}, \binom{-1}{1}, \binom{-1}{-1}$, corresponding function values $0, 1, 0, 1$, and global minimum $\hat{f} - 1$ designed at $\binom{0}{1}$ and $\binom{0}{-1}$.

Acknowledgements

This paper is part of research within the COCONUT project [3], funded by the European Union under the project reference number IST-2000-26063.

References

1. Adjiman, C.S., Dallwig, S., Floudas C.A. and Neumaier, A. (1998), A global optimization method, alphaBB, for general twice-differentiable constrained NLPs – I. *Theoretical advances, Computers and Chemical Engineering* 22, 1137–1158.
2. Brent, R.P. (1973), *Algorithms for Minimization Without Derivatives*, Prentice-Hall, Englewood Cliffs, NJ.
3. COCONUT, COntinuous CONstraints – Updating the Technology, an IST Project funded by the European Union. `http://www.mat.univie.ac.at/~neum/glopt/coconut/index.html`
4. Dixon, L.C.W. and Szegö, G.P. (1978), The global optimization problem: an introduction, in: L.C.W. Dixon and G.P. Szegö (eds.), *Towards Global Optimisation 2*, North-Holland, Amsterdam, pp. 1–15.
5. Kearfott, R.B. (1996), *Rigorous Global Search: Continuous Problems*, Kluwer, Dordrecht.
6. Neumaier, A. (1990), Interval Methods for Systems of Equations, Cambridge Univ. Press, Cambridge.
7. Neumaier, A., Dallwig S. and Schichl, H. (1997), GLOPT – a program for constrained global optimization, in: I. Bomze et al., (eds.), *Developments in Global Optimization*, Kluwer, Dordrecht, pp. 19–36.
8. Pinter, J.D. (1996) *Global Optimization in Action: Continuous and Lipschitz Optimization*, Kluwer, Dordrecht.
9. Ryoo, H.S. and Sahinidis, N.V. (1996), A branch-and-reduce approach to global optimization, *J. Global Optimization* 8, 107–139.
10. Shepard, D. (1965), A two-dimensional interpolation function for irregular spaced data, *Proc. ACM Nat. Conf.* 517–524,
11. Törn, A. and Zilinskas, A. (1989) *Global Optimization, Lecture Notes in Computer Science*, Vol. 350, Springer, Berlin.