Reliable Computing **7:** 497–505, 2001.

A Surprising Approach in Interval Global Optimization

Dedicated to Prof. Dr. Gregory G. Menshikov on the occasion of his 70th anniversary

SERGEY P. SHARY
Institute of Computational Technologies, 630090 Novosibirsk, Russia, e-mail: shary@ict.nsc.ru

(Received: 2 April 2001; accepted: 10 June 2001)

Abstract. The work advances a new class of global optimization methods, called *graph subdivision methods*, that are based on the simultaneous adaptive subdivision of both the function's domain of definition and the range of values.

1. Introduction

The subject matter of our communication is the problem of global optimization of a real-valued function $f : \mathbb{R}^n \supseteq \mathbf{X} \to \mathbb{R}$ over an axis-aligned rectangular box $\mathbf{X}$ (i.e. over an interval vector):

$$\text{find} \quad \min_{x \in \mathbf{X}} f(x). \tag{1.1}$$

The problem (1.1) is known to be (more or less) successfully solved by various interval techniques [1], [2], [4], which enables one to reliably compute two-sided bounds for both the optimum value and the argument it is attained at. The basis of these methods is adaptive, according to the "branch-and-bound" strategy, subdivision of the domain of the function to be minimized combined with the interval evaluation of the ranges over the resulting subdomains.

The purpose of our work is to present a new promising interval approach for the solution of the problem (1.1) that relies upon joint adaptive subdivision of both the function's domain of definition and its range of values. For some classes of problems, the new approach is expected to turn out better than the traditional techniques from [1], [2], [4] in either implementation flexibility or computational efficacy and the quality of the results it produces.

2. Idea of the New Approach

Notice that any function $f : \mathbb{R}^n \supseteq \mathbf{X} \to \mathbb{R}$, being by the very definition a special subset of the direct product $\mathbb{R}^n \times \mathbb{R}$, is an $(n+1)$-dimensional object. In connection

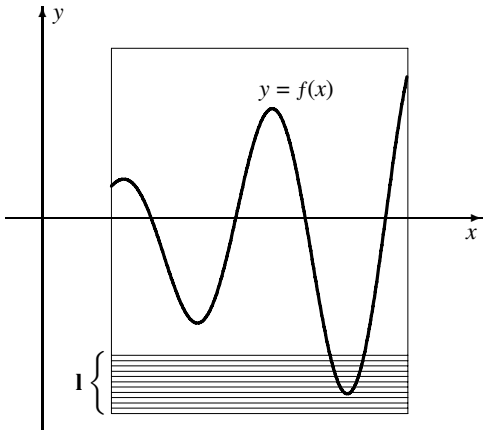

Figure 1. Does the bundle of lines intersect the graph of the function?..

with it, we usually use the concept of the *graph* of the function f. However, the interval global optimization methods that we mentioned in Introduction involve into active operation—adaptive subdivision—only the first n coordinates of this set. The last $(n+1)$-th coordinate of the function represented by its graph is processed in a substantially different manner, passively, and the same is true for the overwhelming majority of the classical optimization techniques. How could we correct the situation and what would be the result?

We start our consideration from the simplest case of a single-variable function $f : \mathbb{R} \supseteq \mathbf{X} \to \mathbb{R}$, defined on a closed interval $\mathbf{X}$, for which we have to solve the problem (1.1). In the plane $0xy$, let us construct a straight line parallel to the first axis, with the equation $y = l$, where l is a constant. We can ascertain whether the line intersects the graph of the function $y = f(x)$ after having solved the equation

$$f(x) - l = 0 \tag{2.1}$$

on $\mathbf{X}$ or, alternatively, making sure that it is incompatible (unsolvable). As is easily seen, the answer to the above question provides us with information on the minimum (1.1) under computation: if the straight line $y = l$ intersects the graph of the function $y = f(x)$, then $\min\limits_{x\in\mathbf{X}} f(x) \le l$. Moreover, if $f(x)$ is continuous on $\mathbf{X}$, then

$$\min_{x\in\mathbf{X}} f(x) = \min\{\, l \in \mathbb{R} \mid \text{ the equation } f(x) - l = 0 \text{ is solvable}\}.$$

Therefore, varying the value of the "level" l and repeating the process of the solution of the equation (2.1), we can substantially improve the estimate for the sought-for minimum (1.1).

The procedure we have just described can be substantially modified by using the ideas and methods of the interval analysis. First, the interval methods make it possible to easily compute estimates for the range of f over $\mathbf{X}$ from below and from

above, which is necessary to determine the bounds of variation of the "level" l in the process of the correction of the minimum. Second, it makes sense to examine the intersection of the graph of the function $y = f(x)$ not with the single lines, but with the whole bundles of lines parallel to the $0x$ axis and defined by the equations $y = \mathbf{l}$, where $\mathbf{l}$ is an interval in $\mathbb{R}$. We will be able thereby to estimate the global minimum (1.1) both from below and from above:

$$\begin{aligned}&\min_{x\in\mathbf{X}} f(x) \text{ is not less than the minimum of the left endpoints and not}\\ &\text{greater than the minimum of the right endpoints of all the intervals } \mathbf{l}\\ &\text{such that the bundle } y = \mathbf{l} \text{ intersects the graph of the function } y = f(x).\end{aligned} \tag{2.2}$$

Third, the interval methods for the solution of equations (e.g. the interval Newton method and its modifications [1]–[3]) enable us, under very mild requirement on the smoothness of f, to examine solvability of both the point equation (2.1) and the interval equation $f(x) - \mathbf{l} = 0$. The latter is understood as the existence of some $l \in \mathbf{l}$ for which (2.1) is solvable.

The answer produced by the interval methods may have one of the following forms [1]–[3]:

1. The equation does not have solutions—*unsolvable*—within the interval under consideration, i.e. $0 \notin f(x) - \mathbf{l}$ for any $x \in \mathbf{X}$.
2. The equation has, with guarantee, a solution (or solutions) within the interval under consideration, i.e. there certainly exists $x^\star \in \mathbf{X}$ such that $f(x^\star) - l = 0$ for at least one $l \in \mathbf{l}$. We shall speak that the equation is just *solvable* then.
3. Applying the solution procedure does not allow us to speak, with certainty, that the equation either has solutions or is unsolvable on the given interval $\mathbf{X}$. In such cases, we shall speak that the equation is *possibly solvable*.

The third option is the most unfavorable algorithmically, but we should carefully take it into account in our reasoning since this kind of uncertainty is quite actual in computation often being the case when the equation (2.1) has multiple roots. Notice also that the interval methods never lose roots and cannot at all output the message "no solutions" if the equation really has them.

Finally, we will use the subdivision of the interval of the range of values instead of the "varying the level" l. The overall interval version of the procedure for finding the global minimum of the single-variable function $f(x)$ over the interval $\mathbf{X}$ can look as follows. It starts with computing a crude interval enclosure $\mathbf{Y}$ of the range of values $f(x)$ over $\mathbf{X}$ (for example, as the natural interval extension of f on $\mathbf{X}$). Further,

- we bisect the interval $\mathbf{Y}$ to beget the subintervals $\mathbf{Y}' := [\underline{\mathbf{Y}}', \operatorname{mid}\mathbf{Y}]$ and $\mathbf{Y}'' := [\operatorname{mid}\mathbf{Y}, \overline{\mathbf{Y}}]$, where $\operatorname{mid}\mathbf{Y} = \frac{1}{2}(\overline{\mathbf{Y}} + \underline{\mathbf{Y}})$ is the midpoint of $\mathbf{Y}$;
- we check the solvability of the interval equations $f(x) - \mathbf{Y}' = 0$ and $f(x) - \mathbf{Y}'' = 0$:
  - if the equation is unsolvable, then we discard the respective interval, either $\mathbf{Y}'$ or $\mathbf{Y}''$, and never consider it;

– solvability or possible solvability of the equation means that either lower or upper estimate of the global minimum can be corrected according to (2.2).

The above procedure correcting the estimate of the minimum (1.1) may be repeated with respect to its descendants $\mathbf{Y}'$ and $\mathbf{Y}''$, after which the bisection-correction ought to be carried out again and so on unless the computed lower and upper bounds of the minimum are not sufficiently close to each other. Notice that, to maintain guarantee of our computation, in such a process we have to keep all the subintervals $\mathbf{y}$ of the initial interval $\mathbf{Y}$ for which the corresponding equations $f(x) - \mathbf{y} = 0$ are possibly solvable, since they may correspond to the bundles having nonempty intersection with the graph.

3. Multidimensional Case

Theoretically, the computational scheme of the one-dimensional global optimization algorithm we have developed in the preceding section is completely applicable to the functions $f(x) := f(x_1, x_2, \ldots, x_n)$ of several variables. The only thing we should be able to do for that is to check intersection of the graph of the function $y = f(x)$ with the bundle of the hyperplanes $y = \mathbf{l}$ that are orthogonal to the $0y$ axis. Sometimes, that can be really done when we have a powerful equations solver and are able to apply it easily. In particular, Semenov [5] implemented a similar kind of procedure to refine the value of the optimum in some problems.

However, in most cases the practical implementation of our idea encounters big difficulties. The point is that, in the general multidimensional case, the solution of an equation—inquiring into its solvability—is in no ways easier problem than the global optimization. As opposed to the single-variable situation, we do not have simple and efficient techniques such as the interval Newton method and its modifications at our disposal. A way out of the difficulty may be subdivision of the domain of definition of f—the box $\mathbf{X}$—along some (but not all!) selected coordinate directions, whose number and specific choice depend on the problem under solution and its objective function.

The coordinate directions along which the function's domain shall not be subdivided will be referred to as *mute*, and first we consider the simplest methods having only one mute direction with the number $\mu \in \{1, 2, \ldots, n\}$. Let, in the space $\mathbb{R}^{n+1}$, a line be given, parallel to the μ-th coordinate axis and having the parametric equation

$$\begin{cases} x_1 = r_1, \\ \quad\vdots \\ x_{\mu-1} = r_{\mu-1}, \\ x_\mu = t, \\ x_{\mu+1} = r_{\mu+1}, \\ \quad\vdots \\ x_n = r_n, \\ y = l, \end{cases} \tag{3.1}$$

where t is a parameter varying over the entire of $\mathbb{R}$ and $r_1, \ldots, r_{\mu-1}, r_{\mu+1}, \ldots, r_n, l$ are some constants. Similar to the one-dimensional case,

$$\min_{x \in \mathbf{X}} f(x) = \min\{\, l \in \mathbb{R} \mid \text{the line (3.1) intersects the graph of the function } y = f(x)\}$$

provided that f is continuous. Therefore, we can "feel about" the graph of the function to be minimized by the one-dimensional lines, making use of the efficient one-dimensional interval procedures (the famous interval Newton method and modifications) to check whether the elementary "level equations" $f(x) - l = 0$ are solvable or not.

Turning to the interval optimization procedure, we designate

$$\mathbf{Z} = (\mathbf{Z}_1, \ldots, \mathbf{Z}_n) := (\mathbf{X}_1, \ldots, \mathbf{X}_{\mu-1}, \mathbf{X}_{\mu+1}, \ldots, \mathbf{X}_n, \mathbf{Y}), \tag{3.2}$$

$$\varphi(\mathbf{Z}, t) := f(\mathbf{X}_1, \ldots, \mathbf{X}_{\mu-1}, t, \mathbf{X}_{\mu+1}, \ldots, \mathbf{X}_n) - \mathbf{Y}. \tag{3.3}$$

The n-dimensional boxes $\mathbf{Z}$ represent the bundles of straight lines parallel to the μ-th coordinate direction and "groping" the graph of the function $y = f(x)$, while the result of either intersection or nonintersection of the bundle with the graph will be determined from the solution of the one-dimensional equation $\varphi(\mathbf{Z}, t) = 0$ on $\mathbf{X}_\mu$ with respect to the unknown t. Keeping all the boxes that have nonempty intersection with the graph is the guarantee that the sought-for global minimum will not be lost.

To sum up, we organize the overall process of the successive improvement of the estimates for the minimum (1.1) similar to what has been done in the popular "branch-and-bound" based interval global optimization techniques from [1], [2], [4]:

- we arrange all the boxes, produced from the subdivision of the initial box $\mathbf{Z}$, as a *working list* $\mathcal{L}$;
- at each step of the algorithm, the bisected box is that from the list $\mathcal{L}$ having the smallest left endpoint of the last component, i.e. the one showing the smallest estimate of the range of f;
- we bisect only the longest component in the box to be subdivided.

Additionally, the boxes of the form (3.2) that the list $\mathcal{L}$ consists of will be ordered so that the values of the left endpoint of their last component (representing the range of values) increase. The first record of the working list is, as usual, called *leading* for the current step of the algorithm. The overall pseudocode of the new method that we are going to call *graph subdivision method* is given in Table 1, where wid means the width of an interval.

Coming up next is a more general situation when s ($1 \leq s \leq n$) coordinate directions are declared as mute, and without loss in generality we can take the

Table 1. The simplest graph subdivision method for global optimization (one mute variable).

Input

A box $\mathbf{X} \subseteq \mathbb{R}^n$ and a function $f : \mathbf{X} \to \mathbb{R}$. An accuracy $\varepsilon > 0$.

A number μ of the mute component, $\mu \in \{1, 2, \ldots, n\}$.

A method for checking the solvability of the single-variable interval equation $\varphi(\mathbf{Z}, t) = 0$ for φ and $\mathbf{Z}$ defined as (3.2)–(3.3).

Output

The lower $\underline{y}$ and upper $\overline{y}$ estimates, with the accuracy ε, for the global minimum of the function f over the box $\mathbf{X}$.

Algorithm

compute an enclosure $\mathbf{Y}$ of the range of f over $\mathbf{X}$;

assign $\mathbf{Z} := (\mathbf{X}_1, \ldots, \mathbf{X}_{\mu-1}, \mathbf{X}_{\mu+1}, \ldots, \mathbf{X}_n, \mathbf{Y})$;

set $z := \underline{\mathbf{Y}}$ and $\overline{y} := \overline{\mathbf{Y}}$;

initialize the working list $\mathcal{L} := \{(\mathbf{Z}, z)\}$;

`DO WHILE` $(\overline{y} - z \geq \varepsilon)$

choose the component k of the box $\mathbf{Z}$ having the largest length, i.e. such that $\operatorname{wid} \mathbf{Z}_k = \max\limits_{1 \leq i \leq n} \operatorname{wid} \mathbf{Z}_i$;

bisect the box $\mathbf{Z}$ along the k-th coordinate to get the boxes $\mathbf{Z}'$ and $\mathbf{Z}''$ such that $\mathbf{Z}' := (\mathbf{Z}_1, \ldots, \mathbf{Z}_{k-1}, [\underline{\mathbf{Z}}_k, \operatorname{mid} \mathbf{Z}_k], \mathbf{Z}_{k+1}, \ldots, \mathbf{Z}_n)$, $\mathbf{Z}'' := (\mathbf{Z}_1, \ldots, \mathbf{Z}_{k-1}, [\operatorname{mid} \mathbf{Z}_k, \overline{\mathbf{Z}}_k], \mathbf{Z}_{k+1}, \ldots, \mathbf{Z}_n)$;

if the equation $\varphi(\mathbf{Z}', t) = 0$ is solvable or possibly solvable on $\mathbf{X}_\mu$, then assign $z' := \underline{\mathbf{Z}}'_n$ and put the record $(\mathbf{Z}', z')$ into $\mathcal{L}$ so that the second fields of the records in $\mathcal{L}$ increase;

if the equation $\varphi(\mathbf{Z}', t) = 0$ is solvable on $\mathbf{X}_\mu$, set $\overline{y} := \min\{\overline{y}, \overline{\mathbf{Z}}'_n\}$;

if the equation $\varphi(\mathbf{Z}'', t) = 0$ is solvable or possibly solvable on $\mathbf{X}_\mu$, then assign $z'' := \underline{\mathbf{Z}}''_n$ and put the record $(\mathbf{Z}'', z'')$ into $\mathcal{L}$ so that the second fields of the records in $\mathcal{L}$ increase;

if the equation $\varphi(\mathbf{Z}'', t) = 0$ is solvable on $\mathbf{X}_\mu$, set $\overline{y} := \min\{\overline{y}, \overline{\mathbf{Z}}''_n\}$;

delete the former leading record $(\mathbf{Z}, z)$ from the list $\mathcal{L}$;

denote the new leading record of the list $\mathcal{L}$ by $(\mathbf{Z}, z)$;

`END DO`

$\underline{y} := z$;

numbers of these directions as $1, 2, \ldots, s$. Let, in the space $\mathbb{R}^{n+1}$, a plane be defined, parallel to the mute coordinate directions and thus determined by the equation

$$\begin{cases} x_1 = t_1, \\ \quad\vdots \\ x_{s-1} = t_{s-1}, \\ x_s = t_s, \\ x_{s+1} = r_{s+1}, \\ \quad\vdots \\ x_n = r_n, \\ y = l, \end{cases} \tag{3.4}$$

where $t_1, \ldots, t_s$ are parameters varying over the whole of the real axis and $r_{s+1}, \ldots, r_n$, l are some constants. Similar to the one-dimensional case, if f is continuous on $\mathbf{X}$,

$$\min_{x \in \mathbf{X}} f(x) = \min\{\, l \in \mathbb{R} \mid \text{the plane (3.4) intersects the graph of the function } y = f(x)\}.$$

We denote

$$\mathbf{Z} = (\mathbf{Z}_1, \ldots, \mathbf{Z}_{n-s+1}) := (\mathbf{X}_{s+1}, \ldots, \mathbf{X}_n, \mathbf{Y}), \tag{3.5}$$

$$\varphi(\mathbf{Z}, t) := f(t_1, \ldots, t_s, \mathbf{X}_{s+1}, \ldots, \mathbf{X}_n) - \mathbf{Y}, \tag{3.6}$$

so as the $(n - s)$-dimensional boxes $\mathbf{Z}$ are bundles of planes of the form (3.4), while either the intersection or nonintersection of such bundles with the graph will be determined from the result of the solution of the interval equation $\varphi(\mathbf{Z}, t) = 0$ with respect to $t = (t_1, t_2, \ldots, t_s)$. Therefore, we can "grope" the graph of the objective function by the planes (3.4) provided that we are able to effectively check the solvability of these equations of s unknowns.

Finally, we arrange the overall process of the successive improvement of the estimates for the global minimum according to the "branch-and-bound" strategy, and the pseudocode of the resulting new algorithm presented in Table 2 is quite similar to the previous case of only one mute direction.

The two pseudocodes are evidently intended for the computation of the function's minimum (1.1) only, but a straightforward modification may adjust the algorithm in order to also find the values of the variables where f takes its global minimums. Namely, we should trace and store all the roots (either certain or possible) of the "level equations" $\varphi(\mathbf{Z}, t) = 0$ apart from the information on their solvability. This will require extending the records comprising the working list $\mathcal{L}$ to incorporate the root enclosures into them.

What can be said about the convergence of the graph subdivision methods? The diameters of the leading boxes are well-known to tend to zero in the classical interval global optimization algorithms from [1], [2], [4], and this should be also valid for the graph subdivision methods inasmuch as their logical structure coincides with

Table 2. The simplest graph subdivision method for global optimization (several mute variables).

Input

A box $\mathbf{X} \subseteq \mathbb{R}^n$ and a function $f : \mathbf{X} \to \mathbb{R}$. An accuracy $\varepsilon > 0$.

A method for checking the solvability of the interval equation $\varphi(\mathbf{Z}, t) = 0$ for $t = (t_1, \ldots, t_s)$ and φ, $\mathbf{Z}$, defined in (3.5)–(3.6).

Output

The lower $\underline{y}$ and upper $\overline{y}$ estimates, with the accuracy ε, for the global minimum of the function f over the box $\mathbf{X}$.

Algorithm

compute an enclosure $\mathbf{Y}$ of the range of f over $\mathbf{X}$;

assign $\mathbf{Z} := (\mathbf{X}_{s+1}, \ldots, \mathbf{X}_n, \mathbf{Y})$;

set $z := \underline{\mathbf{Y}}$ and $\overline{y} := \overline{\mathbf{Y}}$;

initialize the working list $\mathcal{L} := \{(\mathbf{Z}, z)\}$;

DO WHILE $(\overline{y} - z \geq \varepsilon)$

choose the component k of the box $\mathbf{Z}$ having the largest length, i.e. such that $\operatorname{wid} \mathbf{Z}_k = \max\limits_{1 \leq i \leq (n-s+1)} \operatorname{wid} \mathbf{Z}_i$;

bisect the box $\mathbf{Z}$ along the k-th coordinate to half-boxes $\mathbf{Z}'$ and $\mathbf{Z}''$ such that $\mathbf{Z}' := (\mathbf{Z}_1, \ldots, \mathbf{Z}_{k-1}, [\underline{\mathbf{Z}}_k, \operatorname{mid} \mathbf{Z}_k], \mathbf{Z}_{k+1}, \ldots, \mathbf{Z}_{n-s+1})$, $\mathbf{Z}'' := (\mathbf{Z}_1, \ldots, \mathbf{Z}_{k-1}, [\operatorname{mid} \mathbf{Z}_k, \overline{\mathbf{Z}}_k], \mathbf{Z}_{k+1}, \ldots, \mathbf{Z}_{n-s+1})$;

if the equation $\varphi(\mathbf{Z}', t) = 0$ on $(\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_s)$ is solvable or possibly solvable, then assign $z' := \underline{\mathbf{Z}}'_{n-s+1}$ and put the record $(\mathbf{Z}', z')$ into $\mathcal{L}$ so that the second fields of the records in $\mathcal{L}$ increase;

if the equation $\varphi(\mathbf{Z}', t) = 0$ on $(\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_s)$ is solvable, then set $\overline{y} := \min\{\overline{y}, \overline{\mathbf{Z}}'_{n-s+1}\}$;

if the equation $\varphi(\mathbf{Z}'', t) = 0$ on $(\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_s)$ is solvable or possibly solvable, then assign $z'' := \underline{\mathbf{Z}}''_{n-s+1}$ and put the record $(\mathbf{Z}'', z'')$ into $\mathcal{L}$ so that the second fields of the records in $\mathcal{L}$ increase;

if the equation $\varphi(\mathbf{Z}'', t) = 0$ on $(\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_s)$ is solvable, then set $\overline{y} := \min\{\overline{y}, \overline{\mathbf{Z}}''_{n-s+1}\}$;

delete the former leading record $(\mathbf{Z}, z)$ from the list $\mathcal{L}$;

denote the new leading record of the list $\mathcal{L}$ by $(\mathbf{Z}, z)$;

END DO

$\underline{y} := z$;

that of the classical methods. Therefore, the "level equations" $\varphi(\mathbf{Z}, t) = 0$ defined by (3.3) and (3.6) tend to point (noninterval) equations. If the objective function f is such that the roots of $\varphi(Z, t) = 0$ depend continuously on the parameter Z, then we can expect that the graph subdivision method converges to global optimums.

It only remains to mention that the simplest graph subdivision methods have been implemented (using Sun Microsystems' FORTE Fortran) and demonstrated very high sharpness of enclosing the global optimums on a number of the standard test problems, although achieved at the price of relatively large labor consumption. Therefore, much is to be done to modify and tune up the new idea, but this is the subject matter of another papers.

References

1. Hansen, E.: *Global Optimization Using Interval Analysis*, Marcel Dekker, New York, 1992.
2. Kearfott, R. B.: *Rigorous Global Search: Continuous Problems*, Kluwer Academic Publishers, Dordrecht, 1996.
3. Neumaier, A.: *Interval Methods for Systems of Equations*, Cambridge University Press, Cambridge, 1990.
4. Ratschek, H. and Rokne, J.: *New Computer Methods for Global Optimization*, Ellis Horwood, Halsted Press, Chichester, New York, 1988.
5. Semenov, A. L.: Solving Optimization Problems with Help of the UniCalc Solver, in: Kearfott, R. B. and Kreinovich, V. (eds), *Applications of Interval Computations*, Kluwer Academic Publishers, Dordrecht, 1996, pp. 211–225.