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Optimal Multisections in Interval Branch-and-Bound Methods of Global Optimization

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Abstract. In this paper we define multisections of intervals that yield sharp lower bounds in branch-and-bound type methods for interval global optimization. A so called 'generalized kite', defined for differentiable univariate functions, is built simultaneously with linear boundary forms and suitably chosen centered forms. Proofs for existence and uniqueness of optimal cuts are given. The method described may be used either as an accelerating device or in a global optimization algorithm with an efficient pruning effect. A more general principle for decomposition of boxes is suggested.

Key words: Centered form, global optimization, interval branch-and-bound method, optimal lower bound, optimal multisection.

1. Introduction

This paper investigates the question of bisections and more generally of multisections in branch-and-bound methods for global optimization based on interval arithmetic and centered forms of order one. More precisely we consider problems of the type

$$\text{(Pb 1)} \quad \min_{x \in X} f(x)$$

where f is a differentiable function over the real interval X. The global minimum is denoted as f^* and x^* is a global minimizer. Interval arithmetic is used mainly to get an enclosure for the derivative of the function f.

The basic principle of branch-and-bound methods of global optimization consists in splitting intervals into smaller one's so that as many subintervals as possible are removed and then searching for the minimum over the remaining subsets. It is clear that the cutting points play an important role in the convergence of such algorithms. Our main target is to define rules for the choice of cutting points to get the best decomposition of any box $Y \subseteq X$. More precisely, making use of information available during the current step, we search splittings that maximize the lower bound of f^* in the next step and, as much as possible, with a reduced additional cost. It appears that, for a global optimization algorithm, the optimal choice relies upon a *principle of anticipation* which takes into account the underlying bounding method.

Optimal multisections follow from a geometrical interpretation of a generalization of kite inclusion functions [23], the aim of which is initially to get lower bounds of f. Moreover if we consider an increasing number of sections over an interval X we get a strictly monotone increasing sequence of lower bounds converging towards $\inf f(X)$. From this sequence one can built an optimization algorithm but in spite of interesting theoretical properties its numerical efficiency is not proved. This last algorithm can be seen as an extension of classical Lipschitz optimization methods. In this paper we focus our attention mainly on the optimality of cutting points in multisections. Then our method can be used as an accelerating device for branch-and-bound algorithms. In the sequel, the bounding method for global optimization uses centered forms of order one and linear boundary value forms. The same principle may also be applied to other algorithms. The organization of the paper is as follows. In Section 2 we recall how linear centered forms and linear boundary value forms may be used to get lower bounds. We also discuss the principle of the kite algorithm [11, 12]. In this case, looking at an optimal kite, an *a posteriori* interpretation in terms of optimal bisection is given.

Section 3 is devoted, by extending the previous results, to the search of optimal n-sections with the so-called '*generalized kites*'. Then optimal cutting points are obtained from a nonlinear system of equations. Theoretical results about existence, uniqueness, convergence of optimal multisections and some other properties are gathered in Section 4. The proof of existence relies on fixed point theory and affine homotopy. Finally a more general rule for decomposition of boxes is suggested before conclusion.

The following notations and definitions are used:

- $\mathbb{R}$ is the set of reals.
- If X is a finite set, $\operatorname{card} X$ is the number of elements of X.
- If $(a,b)\in\mathbb{R}^2$ then

$$[a,b]=\{x\in\mathbb{R}\colon a\leqslant x\leqslant b\},\quad]a,b[=\{x\in\mathbb{R}\colon a<x<b\}.$$

- If $A\subset\mathbb{R}^n$, $A\neq\emptyset$, then $w(A)=\sup\{\|x-y\|\colon (x,y)\in A\times A\}$, where $\|\cdot\|$ is the Euclidean norm on $\mathbb{R}^n$.
- If φ is a map from X to Y and if $B\subset Y$, then

$$\varphi^{-1}(B)=\{x\in X\colon \varphi(x)\in B\}.$$

- Let Ω be an open bounded subset of $\mathbb{R}^n$, let $\partial\Omega=\overline{\Omega}\setminus\Omega$ be the boundary of Ω and let $\varphi\colon \overline{\Omega}\longrightarrow\mathbb{R}^n$ be a continuous map. Then, for a given $y\in\mathbb{R}^n\setminus\varphi(\partial\Omega)$, one can define the Brouwer *degree*, or *topological degree*, of φ with respect to

Ω and y, denoted $\deg(\varphi, \Omega, y)$. This integer valued function has the following properties:

$$\deg(\varphi, \Omega, y) \neq 0 \Longrightarrow y \in \varphi(\Omega)$$
$$\deg(\varphi - y, \Omega, 0) = \deg(\varphi, \Omega, y)$$
$$\deg(\mathrm{Id}, \Omega, y) = 0 \quad \text{if } y \notin \overline{\Omega},$$

and 1 if $y \in \Omega$; where Id: $\overline{\Omega} \to \mathbb{R}^n$, $\mathrm{Id}(x) = x$. Let h: $\overline{\Omega} \times [0,1] \to \mathbb{R}^n$ be a continuous map, if $y \notin h(\partial\Omega \times [0,1])$ then h is said to be an *admissible homotopy* with respect to y, and we have: $\deg(h_0, \Omega, y) = \deg(h_1, \Omega, y)$ where h_t: $\overline{\Omega} \to \mathbb{R}^n$ is defined by $h_t(x) = h(x,t)$. See, for instance, [3, 15, 22].

2. Kite and Linear Forms

2.1. LINEAR CENTERED FORMS

In interval branch-and-bound methods of global optimization centered forms, Taylor forms are basic tools for finding the bounds or range enclosures of functions. Our study, in this paper, is limited to order one and to the mean value theorem. Linear boundary value forms correspond to the particular case where expansions are centered at extremal points of the interval X. For standard interval arithmetic as well as function evaluations one can refer to Alefeld and Herzberger [1]. Linear boundary value forms (*LBVF* in the sequel) for univariate functions may be found in Neumaier [14] and an extension to the multivariate case in [13]. General branch-and-bound methods for global optimization of interval type are extensively developed in [8, 10, 20].

In problem (Pb 1) let $f \in C^1(X)$ where $X = [a,b]$ and $c \in X$. Let us suppose that $G = [L, U]$ encloses the range of the derivative $f'(X)$ and $L < 0 < U$. Then linear centered forms and linear boundary forms give the following enclosures for the range of f

$$f(X) \subset F_c(X) := [\underline{z}_{cf}, \bar{z}_{cf}] \quad \text{and} \quad f(X) \subset F_{\mathrm{lbvf}}(X, G) := [\underline{z}_{\mathrm{lbvf}}, \bar{z}_{\mathrm{lbvf}}]$$

where $\underline{z}_{cf} := \min\{f(c) + U(a-c),\ f(c) + L(b-c)\}$, $\bar{z}_{cf} := \max\{f(c) + U(b-c),\ f(c) + L(a-c)\}$ and $\underline{z}_{\mathrm{lbvf}} := \inf_X \max\{f(a) + L(x-a),\ f(b) + U(x-b)\}$, $\bar{z}_{\mathrm{lbvf}} := \sup_X \min\{f(a) + U(x-a),\ f(b) + L(x-b)\}$.

2.2. KITE ENCLOSURES

After a splitting of $X = [a,b]$ into $X_1 = [a,c]$ and $X_2 = [c,b]$, linear boundary value forms give the enclosures $F_{\mathrm{lbvf}}(X_1, G_1)$ and $F_{\mathrm{lbvf}}(X_2, G_2)$ where $f'(X_1) \subset G_1$ and $f'(X_2) \subset G_2$. Then a new lower bound for the function f is $\underline{z}_K := \min\{\underline{z}_1, \underline{z}_2\}$

and the upper bound is $\bar{z}_K := \max\{\bar{z}_1, \bar{z}_2\}$. In the following we assume that $G_1 = G_2 := G$. One can see (Figure 1a) that the graph of the function f is enclosed by the two parallelograms linked by the point $C := (u, f(u))$. This figure $K(X, u, G)$ is a so-called '*Kite*' with center C. $F_K(X) := [\underline{z}_K, \bar{z}_K]$ encloses $f(X)$, the range of the function f. Solving problem (Pb 1), we are interested in a center C which gives the best lower bound obtained for $\underline{z}_K^* = \max_{u \in]a,b[}\{\underline{z}_K\}$. Such a point $C^* = (u^*, f(u^*))$ and the associated kite $K(X, u^*, G)$ are said to be optimal and a theorem for existence and uniqueness is given. The purpose of the *Kite algorithm* [11, 12, 23], is to get this optimal center. We give here some properties of kites. Proofs and other properties may be found in [23].

1. $f(X) \subseteq F_K(X)$, for each K
2. $F_K(X) \subseteq F_{\text{lbvf}}(X)$, for each K and G fixed
3. $w(F_K(X)) \to 0$ when $w(X) \to 0$
4. if $Y \subseteq Z$, $Z \subseteq X$ and $F'(Y) \subseteq F'(Z)$ where F' is any inclusion function of the derivative f' then $F_K(Y) \subseteq F_K(Z)$
5. $K(X, u, G_1) \subseteq K(X, u, G_2)$ if $G_1 \subseteq G_2$.

2.3. A POSTERIORI INTERPRETATION OF AN OPTIMAL KITE

In standard interval branch-and-bound methods with bisection the cutting point is $\text{mid}(X) = (a+b)/2$ which is not necessarily an optimal choice even for the symmetrical case $|L| = U$, encountered, for example, with Lipschitz functions. Suppose now that $X = [a, b]$, $X_1 = [a, u]$ and $X_2 = [u, b]$. Let G be the same interval enclosure for the range of the derivatives $f'(X_1)$ and $f'(X_2)$. Suppose that linear boundary value form is used to get lower bounds for the function over X_1 and X_2. Then, if one searches the cutting point which induces the best lower bound, one finds the point u^* that yields the optimal kite over X.

Clearly, the optimal cutting point must change with the underlying bounding technique. For example we could obtain another optimal cutting point u_B^* with the optimal centered form of Baumann [2, 21]. In the next section we consider only lower bounds from linear boundary value forms and optimal kites. The same principle will be applied to multisections as well.

The cutting points obtained above are computed for minimization problems, the optimal cutting points would be different for maximization problems and also if the target is the tightest range enclosure for the function f.

Lipschitz optimization has been extensively studied by Pinter [16], Evtushenko [5, 6] Piyavskii [17] and others. A complete survey by Hansen and Jaumard is in the Handbook of Global Optimization edited by Horst and Pardalos [9].

Here, interval analysis is used mainly to obtain enclosures for the range of the derivative $f'(X)$, denoted by $F'(X)$. This can be done by any method of automatic differentiation with interval arithmetic [7, 18].

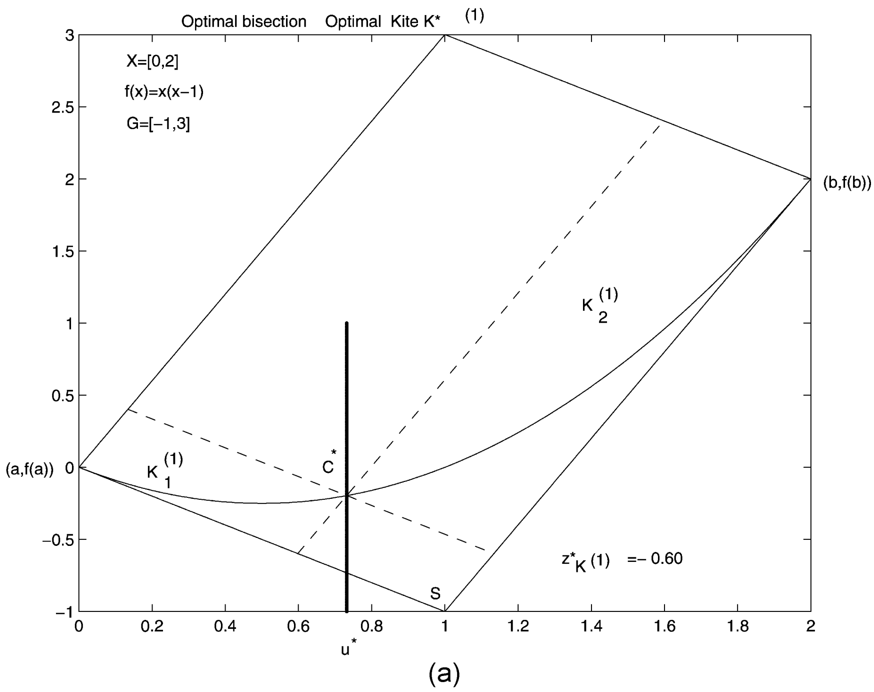

Figure 1a.

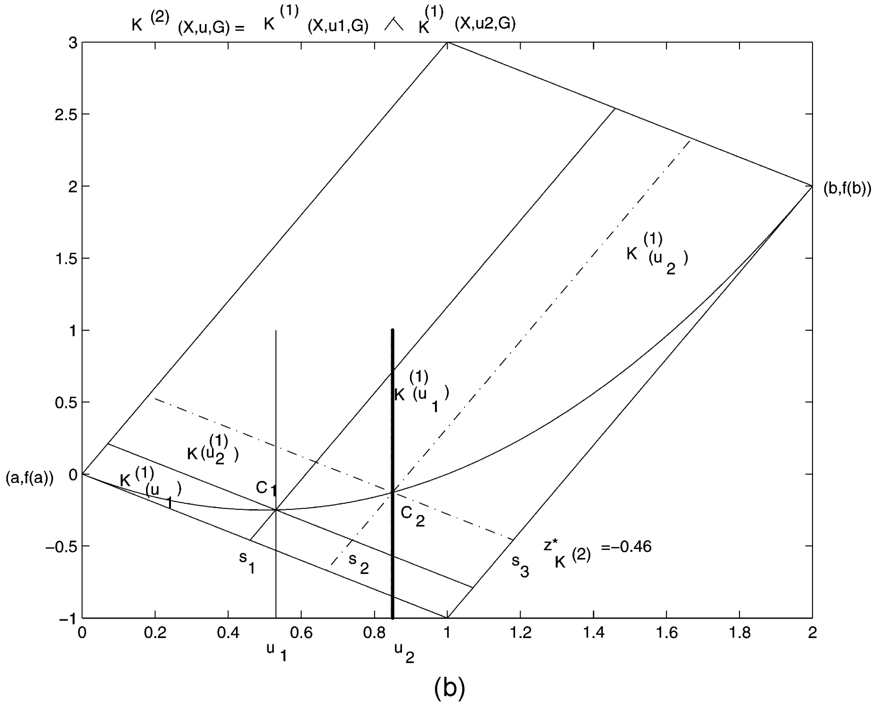

Figure 1b.

3. Multisections and Generalized Kites

3.1. GENERALIZED KITES

In the previous sections a kite is defined as a two-section figure with a single center C. We are now interested, for global optimization problems, in figures with n-sections, $n \geqslant 3$.

For a given function f, let $a < u_1 < u_2 < b$ and $u = (u_1, u_2)^t$. We denote by $K^{(1)}(X, c, G) := K(X, c, G)$ a kite as defined in Section 2. Then we define $K^{(2)}(X, u, G) := K^{(1)}([a, u_2], u_1, G) \cup K^{(1)}([u_1, b], u_2, G)$ as we can see on Figure 1b. More generally let $u = (u_1, u_2, \ldots, u_p)^t$ where $a < u_k < b$ and $u_k < u_{k+1}$ for all k.

DEFINITION 1. Let $u_0 = a$ and $u_{p+1} = b$, the geometrical figure associated to $K^{(p)}(X, u, G) := \cup_{j=1}^{p} K^{(1)}([u_{j-1}, u_{j+1}], u_j, G)$ is called a '*p-center kite*'. This figure is formed with $p+1$-sections linked by the p centers $(u_k, f(u_k))$ and it can be viewed as a generalized kite. Each section is a parallelogram, denoted by $K_k^{(p)}$ resulting from the application of the $LBVF$ method over $X_k = [u_{k-1}, u_k]$.

For X, f and G fixed, a p-center kite (or a *p-kite*, denoted by $K^{(p)}(u)$ for brevity) is related to a splitting of X into $p+1$-sections.

These generalized kites have interesting properties for range enclosure of functions and particularly for lower bounds in global minimization algorithms. Some of these properties are:

1. $\{(x, f(x)), x \in X\} \subseteq K^{(p)}(X, u, G)$ for any $p \geqslant 1$.
2. if $G_1 \subseteq G_2$ then $K(X, u, G_1) \subseteq K(X, u, G_2)$.
3. $K^{(2)}(X, u, G) = K^{(1)}(X, u_1, G) \cap K^{(1)}(X, u_2, G)$.
4. let u be defined as above and $v = (v_1, v_2, \ldots v_q)^t$ with $v_i \neq v_j$ for any i and j, then $K^{(p+q)}(X, s, G) = K^{(p)}(X, u, G) \cap K^{(q)}(X, v, G)$, where $s = (s_1, s_2, \ldots, s_{p+q})^t$, $s_k = u_i$ or v_j and $s_k < s_{k+1}$ for each k.
5. let $F_{K^{(r)}}(X) := [\underline{z}(K^{(r)}), \bar{z}(K^{(r)})]$ be the inclusion function related to the kite $K^{(r)}(X, u, G)$ with $\underline{z}(K^{(r)}) := \min\{\underline{z}_j^{(r)}, j = 1, 2, \ldots, r+1\}$ and $\bar{z}(K^{(r)}) = \max\{\overline{z_j}^{(r)}, j = 1, 2, \ldots, r+1\}$. Then we have the inclusion $f(X) \subseteq F_{K^{(p+q)}}(X) \subseteq F_{K^{(p)}}(X) \cap F_{K^{(q)}}(X)$ for any p and q.

In the next section we will discuss how to use these generalized kites to get sharper lower bounds for a function f.

3.2. OPTIMAL p-KITES

Our aim is now to determine the 'best' p-kite when f, X, and G are given. The question is: can we find a p-kite which gives the best lower bound of the function f? If this one exists, it is defined by $u_* = (u_1^*, u_2^*, \ldots, u_p^*)$ vector of the p centers such that $\underline{z}(K^{(p)}(u_*)) = \sup_u \underline{z}(K^{(p)}(u))$ and this p-kite is said optimal for minimization problem. An optimal u_* satisfies

$$\underline{z}_1^{(p)} = \underline{z}_2^{(p)} = \cdots = \underline{z}_{p+1}^{(p)}$$

with

$$\underline{z}_j^{(p)} = (Uf(u_{j-1}^{(p)}) - Lf(u_j^{(p)}) + (u_j^{(p)} - u_{j-1}^{(p)})LU)\frac{1}{U-L}, \quad j \in \{1,2,\ldots,p+1\} \tag{2}$$

and $u_0 = a$, $u_{p+1} = b$.

Let M and N be the tridiagonal square matrices of order p defined as follows:

$$m_{i,i} := -2 \quad i=1,2,\ldots,p \quad \text{and} \quad m_{i+1,i} = m_{i,i+1} := 1 \qquad i=1,2,\ldots,p-1$$

$$n_{i,i} := -(1/L + 1/U) \qquad i=1,2,\ldots,p$$

$$n_{i+1,i} := 1/L \quad \text{and} \quad n_{i,i+1} := 1/U \qquad \text{for } i=1,2,\ldots,p-1.$$

Let $v = (f(u_1), f(u_2), \ldots, f(u_p))^t$ and $h = \left(-a + \frac{f(a)}{L}, 0, \ldots, 0, -b + \frac{f(b)}{U}\right)^t$. Then u_* is a solution of the nonlinear system $Mu = Nv + h$. In Section 4, we prove that this equation has one solution and that a realistic sufficient condition yields its uniqueness.

3.3. A POSTERIORI INTERPRETATION OF OPTIMAL p-KITES

The first good news is the *existence* and *uniqueness* of a p-kite which yields the best lower bound for f. Moreover if we are looking at a geometrical interpretation of the optimal p-kite (Figure 2), we see that $u_1^*, u_2^*, \ldots, u_p^*$ may be

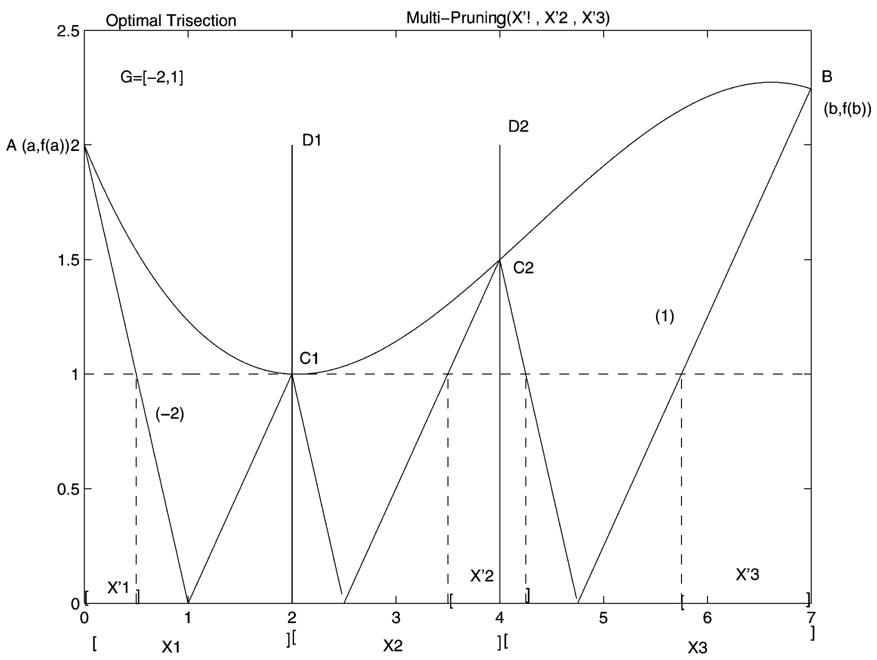

Figure 2.

considered as optimal cutting points for a $p+1$-section of X into $p+1$ subintervals $X_1^*, X_2^*, \ldots, X_{p+1}^*$ when lower bounds are computed by linear boundary value form and G is a same range enclosure for $f'(X_k)$ for each k. Thus the previous interpretation of a standard kite is generalized to any optimal p-kite.

Another good news is that $\underline{z}(K^{(p)}(u_*))$ *converges* towards f^* when $p \to +\infty$. For that reason optimal kites may be included in deterministic algorithms for optimization.

Theoretical results and proofs are gathered in the next section.

4. Theoretical Results

We shall study, without loss of generality, the following 'canonical' case:

$$f \in C^1([0,1]), \quad f(0)=0, \quad f'([0,1]) \subseteq G = [L, U] \quad \text{and} \quad L < 0 < U.$$

Let $\alpha = \frac{1}{L}$, $\beta = \frac{1}{U}$ and $3 \leqslant n$, and assume that the tridiagonal matrices M and N defined in Section 3.2 are associated with linear maps A_n and B_n in $\mathbb{R}^n$ for the basis $\mathcal{B} = \{e_1, e_2, \ldots, e_n\}$ where $(e_i)_j = 1$ if $i = j$ and 0 else. The case $n = 2$ may be studied directly.

The question of existence of an optimal multisection amounts to:

(P_n): can we find $x = (x_1, \ldots, x_n) \in [0,1]^n$ such that $0 < x_1 < \cdots < x_n < 1$ and $A_n(x) = B_n((f(x_1), \ldots, f(x_n))) + (0, \ldots, 0, \beta f(1) - 1)$?

Let $\omega_n = \{x \in]0,1[^n \colon x_1 < x_2 < \cdots < x_n\}$ the open set in $\mathbb{R}^n$ which has for closure the n-simplex $\overline{\omega}_n = \{x \in [0,1]^n \colon x_1 \leqslant x_2 \leqslant \cdots \leqslant x_n\}$, $\partial\omega_n = \{x \in \overline{\omega}_n : (x_1 = 0) \text{ or } (x_n = 1) \text{ or } ((\exists k)(k \in \{1, \ldots, n-1\} \text{ and } x_k = x_{k+1})))\}$.

Let ψ: $\overline{\omega}_n \to \mathbb{R}^n$ be defined with $\psi(x) = B_n((f(x_1), \ldots, f(x_n))) + (0, \ldots, 0, \beta f(1) - 1) - A_n(x)$. Then (P_n) has a positive answer if and only if $\omega_n \cap \psi^{-1}(\{0\}) \neq \emptyset$. The first straightforward but useful result is the

LEMMA 1. *Let* $(a, b) \in [0,1]^2$ *and* $a < b$, *then*:

(1) $\beta(f(b) - f(a)) \leqslant b - a$ *and* $\beta(f(b) - f(a)) = b - a$ *if and only if* $f'([a,b]) = \{U\}$

(2) $-\alpha(f(b) - f(a)) \geqslant a - b$ *and* $-\alpha(f(b) - f(a)) = a - b$ *if and only if* $f'([a,b]) = \{L\}$.

Proof. We have $f(b) - f(a) = \int_a^b f'(t)\mathrm{d}t$ and since $f'([0,1]) \subseteq [L, U]$ we get the classical inequalities $L(b-a) \leqslant f(b) - f(a) \leqslant U(b-a)$. Then the inequalities in (1) and (2) are the result of the fact that $L < 0 < U$. Let any $\tau \in [a,b]$ such that $\varepsilon = U - f'(\tau) > 0$, f' being continuous there is an interval $J \subset [a,b]$ with $\tau \in J$, $l = w(J) > 0$ such that $f'(t) \leqslant U - \varepsilon/2$ if $t \in J$, then $f(b) - f(a) = \int_J f'(t)\mathrm{d}t + \int_{[a,b]\setminus J} f'(t)\mathrm{d}t \leqslant (U - \varepsilon/2)l + U(b - a - l) < U(b-a)$ and thus, equality in (1) is valid if and only if $f'([a,b]) = \{U\}$. The same argument may be used for (2).

LEMMA 2. *Let* $s = (s_1, \ldots, s_n) \in \omega_n$, *then* $\psi(x) \neq \lambda(x - s)$ *for every* $(x, \lambda) \in \partial\omega_n \times]-\infty, 0[$.

Proof. Let $x \in \overline{\omega}_n$, we have

$$\psi_1(x) = -\alpha f(x_1) + \beta(f(x_2) - f(x_1)) + 2x_1 - x_2,$$
$$\psi_k(x) = -\alpha(f(x_k) - f(x_{k-1})) + \beta(f(x_{k+1}) - f(x_k)) - x_{k-1} + 2x_k - x_{k+1}$$
for $k = 2, 3, \ldots, n-1$, and
$$\psi_n(x) = -\alpha(f(x_n) - f(x_{n-1})) + \beta(f(1) - f(x_n)) - x_{n-1} + 2x_n - 1$$

If $x \in \partial\omega_n$ we have the following possibilities:

1. If $x_1 = 0$ then $f(x_1) = f(0) = 0$ thus $\psi_1(x) = \beta f(x_2) - x_2 \leqslant 0$ according to Lemma 1.
   Hence $\psi_1(x) \neq -\lambda s_1$ if $\lambda < 0$ since $s_1 > 0$, and then $\psi(x) \neq \lambda(x - s)$.
2. Let $k \in \{2, \ldots, n-2\}$ such that $x_k = x_{k+1}$. It follows from Lemma 1 that $\psi_k(x) - \psi_{k+1}(x) = -\alpha(f(x_k) - f(x_{k-1})) + x_k - x_{k-1} - \beta(f(x_{k+2}) - f(x_k)) + x_{k+2} - x_k \geqslant 0$. But then $\lambda(x_k - s_k) - \lambda(x_{k+1} - s_{k+1}) = \lambda(s_{k+1} - s_k) < 0$ if $\lambda < 0$ and finally $\psi(x) \neq \lambda(x - s)$ if $\lambda < 0$.
3. If $x_n = 1$ then $\psi_n(x) = -\alpha(f(1) - f(x_{n-1})) + 1 - x_{n-1} \geqslant 0$ by Lemma 1, but $\lambda(x_n - s_n) = \lambda(1 - s_n) < 0$ if $\lambda < 0$, and again $\psi(x) \neq \lambda(x - s)$ if $\lambda < 0$.
4. If $0 < x_1 = x_2$, we get by Lemma 1 $\psi_1(x) - \psi_2(x) \geqslant 0$ and $\lambda(x_1 - s_1) - \lambda(x_2 - s_2) = \lambda(s_2 - s_1) < 0$ if $\lambda < 0$; thus $\psi(x) \neq \lambda(x - s)$ if $\lambda < 0$.

The case $x_{n-1} = x_n < 1$ is treated similarly, and Lemma 2 is proved.

THEOREM 1. $0 \in \psi(\overline{\omega}_n)$.

Proof. Suppose $0 \notin \psi(\partial\omega_n)$, let the homotopy h: $\overline{\omega}_n \times [0,1] \to \mathbb{R}^n$ be defined by $h(x,t) = h_t(x) = (1-t)\psi(x) + t(x - s)$ with $s \in \omega_n$. Obviously h is continuous since ψ is continuous; moreover $0 \notin h(\partial\omega_n \times [0,1])$ because otherwise we could find $(v, \tau) \in \partial\omega_n \times [0,1]$ such that $(1-\tau)\psi(v) = -\tau(v - s)$, but $0 \notin \psi(\partial\omega_n)$ according to the assumption thus $\tau \neq 0$ and $\partial\omega_n \cap \omega_n = \emptyset$, hence $\tau \neq 1$, then $\tau \in]0,1[$ and $\psi(v) = -(\tau/(1-\tau))(v - s)$ which is impossible by Lemma 2. This proves that h is an admissible homotopy related to ω_n and 0; we have $\deg(\psi, \omega_n, 0) = \deg(h_0, \omega_n, 0) = \deg(h_1, \omega_n, 0)$, but $h_1(x) = x - s = (\mathrm{Id} - s)(x)$, so $\deg(h_1, \omega_n, 0) = \deg(\mathrm{Id} - s, \omega_n, 0) = \deg(\mathrm{Id}, \omega_n, s) = 1$ since $s \in \omega_n$. Hence $\deg(\psi, \omega_n, 0) \neq 0$ and $0 \in \psi(\omega_n)$. If $0 \in \psi(\partial\omega_n)$ then finally $0 \in \psi(\overline{\omega}_n)$ which completes the proof.

It should be noted that Theorem 1 does not give a complete answer to (P_n) because if $0 \in \psi(\partial\omega_n)$ we cannot conclude whether $0 \in \psi(\omega_n)$ or not. Actually we have

THEOREM 2. *If $f'^{-1}(\{L, U\})$ does not contain any non empty open interval with extremity 0 or 1 (*), then $\psi^{-1}(\{0\}) \subset \omega_n$, and thus Theorem 1 implies a positive answer to (P_n).*

Proof. We first prove that $\psi(t,t,\dots,t)\neq 0$ for every t in $[0,1]$. This is straightforward from Lemma 1: let $t\in]0,1[$, then $\psi_1(t,t,\dots,t)=-\alpha f(t)+t=0$ and from Lemma 1 $f'([0,t])=\{L\}$ and $]0,t[\subset f'^{-1}(\{L\})$ which is impossible. For $t=0$ and $t=1$ the proofs are similar. Now from this result, if the assumption of Theorem 2 is satisfied, we prove that $u=(u_1,\dots,u_n)\in\partial\omega_n\cap\psi^{-1}(\{0\})$ implies $\operatorname{card}\{u_1,\dots,u_n\}\geqslant 2$. We must consider the cases $u_1=0,\ u_n=1$.

(i) If $u_1=0$, $\operatorname{card}\{u_1,\dots,u_n\}\geqslant 2$ we can find $p\in\{2,\dots,n\}$ such that $u_{p-1}=0<u_p$; then, either $p=2$ and $\psi_1(u)=0$, hence by Lemma 1 $]0,u_2[\subset f'^{-1}(\{U\})$ which contradicts $(^*)$, or $p>2$ and $\psi_{p-1}(u)=0$, which is impossible for the same reason. Therefore $u_1>0$, and by Lemma 1, $u_1<1$ and finally $u_1\in]0,1[$.

(ii) If $u_n=1$, we can find $p\in\{1,\dots,n-1\}$ such that $u_p<u_{p+1}=1$ and by Lemma 1 $f'(]u,1[)=\{L\}$ which contradicts $(^*)$. Then the last case to be examined is: $[u_1,u_n]\subset]0,1[$ and $u_1<u_n$.

Let $p=\min\{k\in\{1,\dots,n-1\}:\ u_k=u_{k+1}\}$. Looking at the different possibilities $p=1$, $p=n-1$, $u_k=u_p$ for all $k>p$, and $u_k=u_{k+1}=\cdots=u_{q-1}<u_q$ with the same previous proof, from Lemma 1 we find in each case a contradiction with $(^*)$. This completes the proof of Theorem 2.

Remarks. Condition $(^*)$ is satisfied when $L<f'(x)<U$ for $x\in]0,1[$ which is often the case if G is computed by interval arithmetic with directed rounding. For $n=2$ trivial modifications in previous proofs yield similar results.

THEOREM 3. *If $f'^{-1}(\{L,U\})$ has no interior point $(^{**})$ is fulfilled, then, for each integer $n\geqslant 2$, there exists one and only one $u\in\overline{\omega}_n$ such that $\psi(u)=0$; moreover $u\in\omega_n$.*

Proof. (1) we prove first that if $(u,v)\in(\psi^{-1}(\{0\}))^2$ then $(u_1=v_1)\Longrightarrow(u=v)$. Actually, if $u_i=v_i$ for $i=1,2,\dots,p$ then $\psi_p(u)-\psi_p(v)=0$ and $u_{p+1}=v_{p+1}$ by Lemma 1 and $(^{**})$ which induces a contradiction if $p\leqslant n-1$.

(2) If $(u,v)\in(\psi^{-1}(\{0\}))^2$ then $u_1<v_1\Longrightarrow u_n>v_n$. We have $\sum_{k=1}^{n}(\psi_k(u)-\psi_k(v))=0$, since $u_1<v_1$ we get from Lemma 1 and $(^{**})$: $\beta(f(v_1)-f(u_1))+u_1-v_1<0$, hence $-\alpha(f(u_n)-f(v_n))+u_n-v_n>0$ and by Lemma 1 $u_n>v_n$.

For one such (u,v) with $u\neq v$, we can suppose by (1) that $u_1<v_1$, and then $\psi_1(u)-\psi_1(v)=0$ which implies, again from Lemma 1, $v_2>u_2$; let $2\leqslant p\leqslant n-1$ and $u_k<v_k$ for $k\in\{1,\dots,p\}$, then $\sum_{k=1}^{p}(\psi_k(u)-\psi_k(v))=0$ yields $v_{p+1}>u_{p+1}$. And finally by induction $u_n<v_n$, which is impossible by Lemma 2.

We can now give a complete answer to the problem of optimal multisection for *LBVF* minimization:

(MAIN) THEOREM 4. *Let $X=[a,b]\subset\mathbb{R}$, let $f\in C^1(X)$ such that $f'(X)\subset[L,U]$ with $LU<0$, and $f'^{-1}(\{L,U\})$ has no interior point, then:*

For each integer $n\geqslant 2$ there is a unique point $u^{(n)}\in X^n$ such that $\psi^{[n]}(u^{(n)})=0$ where $\psi^{[n]}:\{x\in X^n: x_1\leqslant x_2\leqslant\cdots\leqslant x_n\}\longrightarrow\mathbb{R}^n$ is given by $\psi^{[n]}(x)=$

$B_n((f(x_1),\dots,f(x_n)))+(\alpha f(a)-a,0,\dots,0,\beta f(b)-b)-A_n(x)$ *moreover*: $a<u_1^{(n)}<u_2^{(n)}<\cdots<u_n^{(n)}<b$.

Proof. This result is a straightforward generalization of Theorem 3. The choice of $[0,1]$ instead of $[a,b]$ with $f(0)=0$ does not change the proof.

COMPARISON OF $u^{(n)}$ AND $u^{(n+1)}$

One suppose that the assumptions of Theorem 3 are fulfilled.

PROPOSITION 1. *For any integer* $n\geqslant 2$ *the following inequalities hold*: *for any* $k\in\{1,2,\dots,n\}$, $u_k^{(n+1)}<u_k^{(n)}$ *and* $u_n^{(n)}<u_{n+1}^{(n+1)}$.

Proof. (1) $u_1^{(n)}\neq u_1^{(n+1)}$ otherwise from the proof of Theorem 3 part 1) we have $u^{(n)}=(u_1^{(n+1)},\dots,u_n^{(n+1)})$ and $\psi_n^{[n]}(u^{(n)})=0=\psi_n^{[n+1]}(u^{(n+1)})$ and then $\beta(f(1)-f(u_{n+1}^{(n+1)}))-1+u_{n+1}^{(n+1)}=0$ which is impossible according to Lemma 1 and (**).

(2) $n\geqslant 2$ implies that $u_1^{(n+1)}<u_1^{(n)}$.

By (1) we have $u_1^{(n+1)}<u_1^{(n)}$. If we assume that $u_1^{(n)}<u_1^{(n+1)}$ for some n then by proof of Theorem 3, we have: $(\textit{for each } k)(k\in\{1,\dots,n\}\Longrightarrow u_k^{(n)}<u_k^{(n+1)})$ such that: $0=\sum_{k=1}^{n}(\psi_k^{[n]}(u^{(n)})-\psi_k^{[n+1]}(u^{(n+1)}))$ which implies that $\beta(f(1)-f(u_{n+1}^{(n+1)}))+u_{n+1}^{(n+1)}-1>0$, by the fact that $u_n^{(n)}<u_n^{(n+1)}$ and $u_1^{(n)}<u_1^{(n+1)}$ yields: $-\alpha(f(u_n^{(n)})-f(u_n^{(n+1)}))+u_n^{(n)}-u_n^{(n+1)}<0$ and $-\beta(f(u_1^{(n)})-f(u_1^{(n+1)}))+u_1^{(n)}-u_1^{(n+1)}<0$, but this is inconsistent with Lemma 1 and (**).

$u_n^{(n)}<u_{n+1}^{(n+1)}$ is proved as in Theorem 3 with $0=\sum_{k=1}^{n}(\psi_k^{[n]}(u^{(n)})-\psi_k^{[n+1]}\times(u^{(n+1)}))$.

PROPOSITION 2. $\underline{z}_*^{(n)}<\underline{z}_*^{(n+1)}$.

Proof. Again with assumptions of Theorem 3, we have $\underline{z}_*^{(n)}=(-\beta f(u_1^{(n)})+u_1^{(n)})/(\alpha-\beta)$ and $\underline{z}_*^{(n+1)}-\underline{z}_*^{(n)}=(-\beta(f(u_1^{(n+1)})-f(u_1^{(n)}))+u_1^{(n+1)}-u_1^{(n)})/(\alpha-\beta)$. But $u_1^{(n+1)}<u_1^{(n)}$ by Proposition 1 and by Lemma 1, $z_*^{(n)}-\underline{z}_*^{(n+1)}<0$, because $\alpha-\beta<0$.

PROPOSITION 3. $\underline{z}_*^{(n)}\longrightarrow f^*$ *when* $n\longrightarrow+\infty$.

Proof. $(\underline{z}_*^{(n)})_{n\geqslant 2}$ is an increasing sequence by Proposition 2, obviously bounded by $\min f(X)$, hence convergent. If $\underline{z}$ denotes the limit of the sequence, then $\underline{z}\leqslant\min f(X)$.

Let $\rho_n=\min\{u_{k+1}^{(n)}-u_k^{(n)};k=0,1,\dots,n\}$ where $u_0^{(n)}=a$ and $u_{n+1}^{(n)}=b$. It is an obvious geometrical fact that a number $\theta>0$, function only of L and U, exists such that: $w(K_k^{(n)}(u_*))\leqslant\theta\|(u_k^{(n)},\ f(u_k^{(n)}))-(u_{(k+1)}^{(n)},\ f(u_{(k+1)}^{(n)}))\|$ thus $w(K_k^{(n)}(u_*))\leqslant\theta(1+(L-U)^2)^{1/2}(u_{k+1}^{(n)}-u_k^{(n)})$. Let $k(n)$ such that $\rho_n=u_{k(n)+1}^{(n)}-u_{k(n)}^{(n)}$, then: $w(K_k^{(n)}(u_*))\leqslant\theta(1+(L-U)^2)^{1/2}\rho_n\leqslant\theta(1+(L-U)^2)^{1/2}(b-a)/(n+1)$, hence $f(u_{k(n)}^{(n)})-\underline{z}_*^{(n)}\leqslant w(K_{k(n)}^{(n)}(u_*))$ and $\min f(X)-\underline{z}_*^{(n)}\leqslant\theta(1+(L-U)^2)^{1/2}(b-a)/(n+1)\longrightarrow 0$ when $n\longrightarrow+\infty$.

There is now to prove that the multisection resulting from the main theorem is really the optimal one related to *LBVF* minimization. Indeed if $v=(v_1,\dots,v_n)\in[a,b]^n$ is such that $v_1\leqslant v_2\leqslant\cdots\leqslant v_n$ then if $p=\mathrm{card}\{v_1,\dots,v_n\}$, we can consider the p-center kite $K^{(p)}(v_*)$. If we assume now that $\underline{z}_k^{(p)}\geqslant\underline{z}_*^{(p)}$ for each k then, as in proof of Proposition 1 we must have: $v_1\leqslant u_1^{(p)}, v_2\leqslant u_2^{(p)},\dots,v_p\leqslant u_p^{(p)}$. In fact we assume that $\{v_1,\dots,v_n\}=\{v_1,\dots,v_p\}$, with a new numbering if necessary. According to this result we get $v_p<u_p^{(p)}\Longrightarrow\underline{z}_p^{(p)}<\underline{z}_*^{(p)}$ which is impossible, therefore: $u_p^{(p)}\leqslant v_p$, thus $u_p^{(p)}=v_p$ and for analogous reasons $u_k^{(p)}=v_k$ for each $k\in\{1,\dots,p\}$. Then the proof is achieved from Proposition 2 because $\underline{z}_*^{(p)}\leqslant\underline{z}_*^{(n)}$. Proposition 1 and Proposition 2 remain true for any interval $X=[a,b]$ without any assumption about $f(a)$ and finally we have proved the following:

(MAIN) THEOREM 5. *Let $X=[a,b]$ a proper interval of $\mathbb{R}$, $f\in C^1(X)$ such that $f'(X)\subseteq[L,U]$, $LU<0$. If $f'^{-1}(\{L,U\})$ has no interior point, then the following holds*:

For every integer $n(n\geqslant 2)$, there is one and only one n-center kite related to LBVF minimization $K_*^{(n)}=K^{(n)}(X,u^*,G)$ which satisfies

(1) *$a<u_1^*<\cdots<u_n^*<b$ and $\underline{z}_k^{(n)}=\underline{z}_*^{(n)}$ for each $k\in\{1,\dots,n\}$.*
(2) *$K_*^{(n)}$ is the best n-center kite related to LBVF minimization.*

Moreover we have: *$\underline{z}_*^{(n)}<\underline{z}_*^{(p)}$ if $n<p$ and $\underline{z}_*^{(n)}\longrightarrow f^*$ when $n\longrightarrow+\infty$.*

Not only does (Main) Theorem 5 bring existence and uniqueness of an optimal multisection but it also yields, from a recursive computation of the sequence $(K_*^{(n)})$, a *new algorithm* for solving a global optimization problem with its optimizers, since at each step we get a narrower enclosure for f^*.

The following properties may be used for the computation of the centers of optimal n-kites.

PROPOSITION 4. *The centers $(v_k^*,\ f(v_k^*))$ are enclosed in $K_*^{(n)}$ and every section $K_{k*}^{(n)}$ contains one and only one center of $K_*^{(n+1)}$.*

Proof. The centers of $K_*^{(n+1)}$ are points of graph$(f(X))$ which is enclosed in any kite and therefore in $K_*^{(n)}$. The number of sections $K_{k*}^{(n)}$ of $K_*^{(n)}$ is equal to the number of centers of $K_*^{(n+1)}$. Then if two centers of $K_*^{(n+1)}$ are in the same section of $K_*^{(n)}$, one section $K_{j*}^{(n)}$ of $K_*^{(n)}$ does not contain any center of $K_*^{(n+1)}$. Let $C_i^*=(v_i^*,\ f(v_i^*))\in K_{j-1*}^{(n)}$ and $C_{i+1}^*=(v_{i+1}^*,\ f(v_{i+1}^*))\in K_{j+1*}^{(n)}$.

The lowest point of $K_*^{(n+1)}$ in $[u_i,u_{i+1}]$ of coordinates $(\underline{x}_i^*,\underline{z}_*^{(n+1)})$ is such that $\underline{z}_*^{(n+1)}<\underline{z}_*^{(n)}$, which is in contradiction with Proposition 2. Actually, $\underline{z}_{k*}^{(p)}<\underline{z}_*^{(p)}$ for every k and p, moreover if u^* is the vector of the abscissa of centers of $K_*^{(n)}$, $(U-L)(z_{i*}^{(n+1)}-z_{j*}^{(n)})=U(f(v_i^*)-f(u_{j-1}^*))-L(f(v_{i+1}^*)-f(u_j^*))+LU((v_{i+1}^*-u_j^*)-(v_i^*-u_{j-1}^*))<0$ because $f'(X)\subseteq[L,U]$, $v_{i+1}^*>u_j^*$ and $v_i^*<u_{j-1}^*$.

The result is *a fortiori* true if a section of $K_*^{(n)}$ contains more than two centers of $K_*^{(n+1)}$.

The next result gives complementary information about the sequence $(K_*^{(n)})$ and completes Proposition 1.

PROPOSITION 5. *Let $X=[a,b]$, let $K_*^{(n)}$ and $K_*^{(n+1)}$ be two optimal consecutive kites, let $(\underline{x}_i^{*(p)},\ \underline{z}_*^{(p)})$ be the lowest point of $K_*^{(p)}$, $i=1,\dots,p+1$ and assume that the condition $(^{**})$ of Theorem 3 is satisfied. Then the cutting points of $K_*^{(n)}$ separate the cutting points of $K_*^{(n+1)}$:*

$$(^{***}) \qquad a<\cdots<u_i^{*(n+1)}<u_i^{*(n)}<u_{i+1}^{*(n+1)}<\cdots<b.$$

Moreover $(\underline{x}_i^{*(n+1)},\ \underline{z}_*^{(n+1)})\notin K_*^{(n)}$ and $(^{****})$ $\underline{x}_i^{*(n+1)}<\underline{x}_i^{*(n)}<\underline{x}_{i+1}^{*(n+1)}$, $i=1,\dots,n$.

Proof. $(^{***})$ is straightforward from Proposition 4 because any section of $K_*^{(n)}$ delimited by two consecutive centers contains a single center of $K_*^{(n+1)}$. If $(\underline{x}_i^{*(n+1)},\ \underline{z}_*^{(n+1)})$ is inside $K_*^{(n)}$, this one must contain at least two centers of $K_*^{(n+1)}$, which is excluded. Inequalities $(^{****})$ may be verified directly: $\underline{x}_i^{(n+1)}<\underline{x}_i^{(n)} \Longleftrightarrow f(u_{i-1}^{(n+1)})-f(u_i^{(n+1)})+Uu_i^{(n+1)}-Lu_{i-1}^{(n+1)}<f(u_{i-1}^{(n)})-f(u_i^{(n)})+Uu_i^{(n)}-Lu_{i-1}^{(n)} \Longleftrightarrow (u_{i-1}^{(n+1)}-u_{i-1}^{(n)})(f'(\xi)-L)+(u_i^{(n+1)}-u_i^{(n)})(U-f'(\eta))<0$, but $f'(x)\in[L,U]$ and $u_j^{(n+1)}<u_j^{(n)}$. Therefore equality is impossible. The proof of the second inequality is analogous.

These properties are very useful for the computation of optimal centers by iterative interval methods.

EXAMPLE. We can see on Figures 1a and b optimal kites for bisection and trisection when the function $f(x)=x^2-x$ with $X=[0,2]$ and $G=[-1,3]$. In Table 1 we give, for some values of n, lower bounds obtained with uniform mesh and $n-1$-kites; moreover $\underline{z}_{\text{lbvf}}=-1$ and $f^*=-0.25$.

5. Applications

5.1. ACCELERATING DEVICE

When optimal *p-kites* are used to determine optimal cutting points for $p+1$-*sections* according to assumptions given in Section 3.2, then the integer p has a *fixed* value. If p is too large, an accurate and guaranteed computation may be very

Table 1.

n	2	3	4	5	6	11
Uniform n-Sections	−0.75	−0.5556	−0.5625	−0.5200	−0.4722	−0.3719
Optimal n-Sections	−0.60	−0.4590	−0.3910	−0.3530	−0.3294	−0.2802

expensive. Actually one must find the single solution of the nonlinear equation $\psi(u) := Mu - N\nu - h = 0$. The nonlinearity is localized in $\nu = (f(u_1), \ldots, f(u_p))^t$. This equation can be solved by point or interval Newton-like methods.

For an iterative Newton-like method, if u is the current value, the next one u^+ is computed by solving the linear system $J_\psi(u)(u^+ - u) = -\psi(u)$ where $J_\psi(u) := M - N\mathrm{diag}(f'(u_1),\ f'(u_2), \ldots, f'(u_p))$. One iteration step involves p point evaluations of $(f(u), f'(u))$ and the resolution of tridiagonal linear system of order p. The amount of evaluations may be reduced by the use a parallel chord method. For an interval method the fixed matrix $A = M - GN$ could be used instead of J_ψ. Moreover if the target is only an improved splitting, the optimal solution is not necessary and a few number of iterations will be sufficient. Then the method described above must be seen as an heuristic tool that may be added to other accelerating devices for global interval optimization. The framework is then

Algorithm Selecting cutting points

Step 1. Let p have a fixed value. Select an interval $Y = [\underline{y}, \bar{y}]$ in the working list $\mathcal{L}$. Let $u_0^+ := \underline{y}$ and $u_{p+1}^+ := \bar{y}$.
Step 2. Apply a point or interval method that yields an approximate solution u^+ of $\psi(u) = 0$.
Step 3. Delete Y from the working list $\mathcal{L}$, continue the global optimization algorithm over the intervals $Y_k = [u_{k-1}^+, u_k^+]$, for $k = 1, 2, \ldots, p+1$.

5.2. p-KITES AS GLOBAL OPTIMIZATION ALGORITHM

One first notices that using the lowest point of *generalized kites* as a bounding rule is quite similar to saw-tooth methods in Lipschitz optimization. Thus our method could be interpreted as a slight generalization of Lipschitz methods with $|L| \neq U$. But the main difference is that, for *p-kites*, the points $u_k^{(n)}$ are not computed sequentially but simultaneously to get $\underline{z}_*^{(p)}$.

We know from Theorem 5 that $\underline{z}_*^{(n)}$ converges monotonically towards f^* when $n \to +\infty$ and, according to Proposition 5, good initial values are available at each step. Unfortunately the resolution of the non linear system has also an increasing cost. We do not deal with this aspect of *p-kites* in this paper, but a good strategy could consist in working with a fixed value of p over an interval Y, then computing enough accurately the optimal cutting points. Subsets Y_k' which cannot contain minimizers will be discarded by applying a pruning rule [12]. As can be seen in the example given Figure 2 for intervals X_k', the pruning results from the intersection of the boundary of the *p-kite* with the horizontal line $t = \min f(u_j^{(p)})$. The process will be applied again over the remaining subboxes updating enclosures of the derivative for a better efficiency.

6. Conclusion

A new method for enclosing the graph of univariate real functions inside geometrical figures, so called *generalized kites*, has been presented. This paper focuses principally on the cutting points of multisections. An algorithm is developed that allows to define optimal multisections, for information available at the current step, in interval branch-and-bound methods of global optimization using linear under bounds. Theoretical results concerning existence, uniqueness and convergence are given. As an immediate application of the method, the *generalized kites* can be used as an accelerating device choosing better cutting points that are then roughly localized. Thus a new rule can be combined with tools for selecting a box or choosing a direction for splitting. These devices are built on properties of the function and geometrical dimensions of the box, the rule defined in this paper is closely related to the bounding technique. Another application would be to use recursively *p-kites* building thus a branch-and-bound type algorithm of global optimization but this point is not studied here.

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