Efficient combination of two lower bound functions in univariate global optimization

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Abstract. We propose a new method for solving univariate global optimization problems by combining a lower bound function of αBB method (see [1]) with the lower bound function of the method developed in [4]. The new lower bound function is better than the two lower bound functions. We add the convex/concave test and pruning step which accelerate the convergence of the proposed method. Illustrative examples are treated efficiently.

Keywords. Global optimization, αBB method, quadratic lower bound function, Branch and Bound, pruning method.

1 Introduction

We consider the following problem

$$(P) \begin{cases} \min b(s) \\ s \in [s^0, s^1] \subset R \end{cases}$$

with f of class C^2 and nonconvex on $[s^0, s^1]$ an interval of R.

Several methods have been studied in the literature for univariate global optimization problems. Let us mention some works, in [5] a branch and prune algorithm is proposed, the pruning step(outer and inner) consists in solving linear equation, the linear bounding function is obtained by interval analysis. In [3] a branch and bound algorithm is presented for Holder functions. In [6], the improved linear bounding function is used and discard regions which do not contain the minimum global by the pruning step(outer) as in [5]. In [2] a review of recent advances in global optimization is presented.

Univariate global optimization problems attract attention of researchers not only because they arise in many real-life applications but also the methods for these problems are useful for the extension for the multivariable case or by reducing the multidimensional case to the univariate case. One class of deterministic approaches, which called lower bounding method, emerged from the natural strategy to find a global minimum for sure. The efficiency of a method is in the construction of tight lower bound and to discard a big regions which do not contain the global minimum as quickly as possible.

The aim of this paper is to combine the lower bound function of the method

which was already proposed (see [1]) with the lower bound function of the method developed in [4] by constructing a better lower bound function. The convergence is accelerated by adding the convex/concave test and the pruning step, this is done by using the parameters of the two methods and by solving quadratic equations respectively.

The structure of the paper is as follows. The two lower bound functions in [1] and in [4] with their properties are presented in section 2. In section 3, a new lower bound is stated. In section 4, the algorithm is described and its convergence is shown. Section 5 presents illustrative examples.

2 Background

2.1 Lower bound in αBB method

The lower bound in αBB method on the interval $[s^0, s^1]$ is

 $LB_{\alpha}(s) = b(s) - \frac{K_{\alpha}}{2}(s-s^0)(s^1-s)$ with $K_{\alpha} = max\{0, -\underline{b^{\prime\prime}}\}$ such that $\underline{b^{\prime\prime}} \leq b^{\prime\prime}(s), \forall s \in [s^0, s^1]; \underline{b^{\prime\prime}}$ is obtained by the interval analysis method.

The properties of this lower bound function are:

1/ It is convex (i.e. $LB''_{\alpha}(s) = b''(s) + K_{\alpha} = b''(s) + max\{0, -\underline{b''}\} \ge b''(s) - \underline{b''} \ge 0, \forall s \in [s^0, s^1]$).

2/ It coincides with the function b at the end points of the interval $[s^0, s^1]$ (i.e. by construction of $LB_{\alpha}(s)$).

3/ it is a lower bound function (i.e. $b(s) - LB_q(s) = \frac{K_{\alpha}}{2}(s-s^0)(s^1-s) \ge 0, \forall s \in [s^0, s^1]$).

For details see [1].

2.2 Quadratic lower bound

The quadratic lower bound developed in [4] on the interval $[s^0, s^1]$ is $LB_q(s) = b(s^0) \frac{s^{1-s}}{s^{1-s^0}} + b(s^1) \frac{s-s^0}{s^{1-s^0}} - \frac{K_q}{2}(s-s^0)(s^1-s)$ with $K_q = max\{0, \overline{b''}\}$ such that $\overline{b''} \ge b''(s), \forall s \in [s^0, s^1]; \overline{b''}$ is obtained by the interval analysis method.

The properties of this lower bound function are:

1/ It is convex (i.e. $K_q \ge 0$).

2/ It coincides with the function b at the end points of the interval $[s^0, s^1]$ (i.e. by construction of $LB_q(s)$).

3/ it is a lower bound function (i.e. $(b(s) - LB_q(s))^{"} = b^{"}(s) - K_q = b^{"}(s) - max\{0, \overline{b^{"}}\} \leq b^{"}(s) - \overline{b^{"}} \leq 0$ which implies that $(b(s) - LB_q(s))$ is concave, it vanishes at the end points of $[s^0, s^1]$ then $b(s) - LB_q(s) \geq 0, \forall s \in [s^0, s^1]$. For details see [4].

Lemma 1. The second derivative of b is bracketed between $-K_{\alpha}$ and K_q (i.e. $-K_{\alpha} \leq b^{"}(s) \leq K_q, \forall s \in [s^0, s^1]$).

Proof. One has $K_{\alpha} = max\{0, -\underline{b}^n\} \ge -\underline{b}^n \Rightarrow -K_{\alpha} \le \underline{b}^n$ then $-K_{\alpha} \le \underline{b}^n \le b^n(s), \forall s \in [s^0, s^1]$ and the first inequality is proved. The second inequality is immediate.

New lower bound function 3

We now present the new lower bound function on the interval $[s^0, s^1]$, LB(s) = $max\{LB_{\alpha}(s), LB_{a}(s)\}$

Its properties are:

1/LB(s) is convex on the interval $[s^0, s^1]$ because it is a maximum of convex functions on the interval $[s^0, s^1]$.

2/ It coincides with the objective function at the end points of the interval $[s^0, s^1]$ by construction.

3/ It is a lower bound function and better than the two lower bound $LB_{\alpha}(s)$ and $LB_q(s)$ by construction

Remark 1. This new lower bound is nonsmooth function, to compute its minimum, we can use the subgradient method or solve the following convex problem

$$\begin{cases} \min z \\ LB_{\alpha}(s) \leq z \\ LB_{q}(s) \leq z \\ s \in [s^{0}, s^{1}], z \in R \end{cases}$$

Convex/concave test 3.1

At iteration k we compute K_q^k and K_{α}^k on the interval $[a_k, b_k]$ by the interval analysis method.

By the inequalities $-K_{\alpha} \leq b^{"}(s) \leq K_{q}, \forall s \in [s^{0}, s^{1}]$ (see lemma 1), one has i) If $K_{\alpha}^{k} = 0$ (i.e. $0 \leq b^{"}(s), \forall s \in [s^{0}, s^{1}]$) then b is convex on the interval $[a_{k}, b_{k}]$, any local search gives a global minimum on this interval ii) If $K_q^k = 0$ (i.e. $b^{"}(s) \leq 0, \forall s \in [s^0, s^1]$) then b is concave on the interval $[a_k, b_k]$

and its minimum is attained at the end point of this interval.

Remark 2. The algorithm may stop by the convex/concave test if it is satisfied for all subintervals.

Pruning method 3.2

 $LB_q^k(s)$ the quadratic lower bound on the interval $[a_k, b_k]$ and UB_k the current upper bound in the Branch and prune algorithm.

We solve the quadratic equation $LB_q^k(s) = UB_k$,

we have three cases:

1/ There is no solution then the entire interval $[a_k, b_k]$ is fathomed.

2/ There is a double solution, if the value of the objective function at this solution is equal to UB_k , the interval is reduced to one point(this solution) and we actualize the upper bound else the entire interval $[a_k, b_k]$ is fathomed.

3 There is two distinct solutions $a_k^{r_1}$ and $b_k^{r_1}$ then the interval $[a_k, b_k]$ is reduced to $[a_k^{r_1}, b_k^{r_1}]$

We compute again $LB_q^k(s)$ on the interval $[a_k^{r_1}, b_k^{r_1}]$ we solve the quadratic equation $LB_q^k(s) = UB_k$ and see the above three cases We repeat this procedure until $b(a_k^{r_j}) = b(b_k^{r_j}) = UB_k$.

Remark 3. If the optimal solution is found at iteration k and the stopping rule $UB_k - LB_k < \varepsilon$ isn't satisfied, the pruning method allows us to confirm this solution and to stop the algorithm.

We present two simple examples. Example 1 $b(s) = -s^3 + s^2, s \in [0, 2]$ $b''(s) = -6s + 2, -10 \le b''(s) \le 2, K_q = 2, K_\alpha = 10$ $LB_q(s) = s^2 - 4s$ $, LB_\alpha(s) = -s^3 + 6s^2 - 10s$ The minimum of $LB_q(s)$ is attained at s = 2 and then is the global minimum of the objective function. The minimum of $LB_\alpha(s)$ is attained at the point $s = 2 - \frac{\sqrt{3}}{3}$ which is not the global minimum of the objective function

For this example $LB_q(s)$ is better than $LB_{\alpha}(s)$.

Remark 4. If we take $b(s) = s^3 - s^2, s \in [0, 2]$ $K_q = 10, K_\alpha = 2$ $LB_\alpha(s)$ is better than $LB_q(s)$.

Example 2 $f(s) = sins + coss, s \in [0, 2\pi]$ $f''(s) = -sins - coss; -2 \leq f''(s) \leq 2; K_{\alpha} = K_q = 2,$ $LB_q(s) = 1 - s(2\pi - s); LB_{\alpha}(s) = sins + coss - s(2\pi - s)$ The minimum of $LB_q(s)$ is attained at $s = \pi$, and $LB_q(\pi) = -1 - \pi^2$. The minimum of $LB_{\alpha}(s)$ is attained at the point $s = \frac{9\pi}{8}$, and $LB_{\alpha}(\frac{9\pi}{8}) = -1, 3 - \pi^2$. For this example $LB_q(s)$ is better than $LB_{\alpha}(s)$.

Remark 5. By using LB(s), we are sure that this lower bound function is always better than the two lower bound functions $LB_{\alpha}(s)$ and $LB_{q}(s)$.

4 Algorithm and its convergence

We now describe the algorithm

4.1 Algorithm

1.Initialization:

a) Let ε be a given sufficiently small number, let $[s^0, s^1]$ the initial interval,

compute K^0_{α} and K^0_a such that $K^0_{\alpha} = max\{0, -\frac{1}{2}\overline{b}^n\}$, and $K^0_a = max\{0, \frac{1}{2}\overline{b}^n\}$ with \overline{b} " a upper bound of b"(s) on [s⁰, s¹]. b)Convex/concave test If $K^0_{\alpha} = 0$ stop b is convex, any local search gives an optimal solution. If $K_q^0 = 0$ stop b is concave, the optimal solution is attained on the end point of $[s^0, s^1]$ Else c)Pruning step if $b(s^0) = b(s^1)$ no pruning else compute LB_q^0 and solve the equation $LB_q^0 = min\{b(s^0), b(s^1)\}$ to obtain $[s^{0r_1}, s^{1r_1}].$ Compute $LB_q^{r_1}$ and solve the equation $LB_q^{r_1} = min\{b(s^0), b(s^1)\}$ to obtain $[s^{0r_2}, s^{1r_2}].$ Repeat this procedure until $b(s^{0r_j}) = b(s^{1r_j}) = \min\{b(s^0), b(s^1)\}$ e)Set $k := 0; T^0 = [a_0, b_0] := [s^{0r_j}, s^{1r_j}]; M := T^0$ f)Compute $LB^0_{\alpha}(s)$ and $LB^0_q(s)$ on T^0 , and solve the convex program $\min \left\{ z : LB^0_{\alpha}(s) \leq z, LB^0_q(s) \leq z, z \in \mathbb{R}, s \in T^0 \right\}$ to obtain an optimal solution z^0 and s^0_0 . g)Set $UB_0 := \min \{ b(a_0), b(b_0), b(s_0^*) \} = b(\overline{s}^0), \ LB_0 = LB(T^0) := z^0.$ 2. While $UB_k - LB_k \ge \varepsilon$ do 3. Let $T^k = [a_k, b_k] \in M$ be the interval such that $LB_k = LB(T^k)$ 4.Bisect T^k into two intervals by w - subdivision procedure $\begin{array}{l} T_1^k = [a_k, s_k^*]; T_2^k = [s_k^*, b_k] \\ \text{Set } T_1^k := [a_k^1, b_k^1] \text{ and } T_2^k := [a_k^2, b_k^2] \end{array}$ 5. For i = 1, 2 do a) Convex/concave test Compute K_{α}^{ki} and K_{q}^{ki} on T_{i}^{k} . If $K_{\alpha}^{ki} = 0$, b is convex, any local search gives an optimal solution s_{ki}^* on T_i^k , then update $LB(T_i^k) = UB(T_i^k) = b(s_i^k)$ and goto 5.d) If $K_a^{ki} = 0$ b is concave on T_i^k , then update $LB(T_i^k) = UB(T_i^k) = min\{b(a_k^i, b(b_k^i))\}$ and goto 5.d) b) Pruning step Compute LB_{q}^{ki} and solve the equation $LB_{q}^{ki} = UB_{k}$ to obtain $T_i^{kr_1} = [a_{kr_1}^i, \dot{b}_{kr_1}^i],$ Compute $LB_q^{kr_1i}$ and solve the equation $LB_q^{kr_1i} = UB_k$ to obtain $T_i^{kr_2} = [a_{kr_2}^i, b_{kr_2}^i],$ Repeat this procedure until $b(a_{kr_i}^i) = b(b_{kr_i}^i) = UB_k$ Set $T^k_i = [a^i_k, b^i_k] := [a^i_{kr_i}, b^i_{kr_i}]$ c)Compute $LB^{ki}_{\alpha}(s)$ Set s_{ki}^* the solution of the convex problem $\min \left\{ z : LB_{\alpha}^{ki}(s) \leq z, LB_{q}^{ki}(s) \leq z, z \in R, s \in T_{i}^{k} \right\}$ d) To fit into *M* the intervals $T_{i}^{k} : M \leftarrow M \bigcup \{T_{i}^{k} : UB_{k} - LB(T_{i}^{k}) \geq \varepsilon, i =$

1,2} \ { T^k } e) Update $UB_k = min\{UB_k, b(a_k^i), b(b_k^i), b(s_k^{*i})\} := b(\overline{s}^k)$ 6. Update $LB_k = min\{LB(T) : T \in M\}$ 7. Delete from M all intervals T such that $LB(T) > UB_k - \varepsilon$. 8. Set k := k + 19. End while 10. \overline{s}^k is an ε - optimal solution to (P)

4.2 Convergence

Theorem 1. The sequence $\{\overline{s}^k\}$ generated by the algorithm converges to an optimal solution of the problem (P)

Proof. If the algorithm stops at iteration k which may be obtained by the convex/concave test or the pruning method or the stopping rule $UB_k - LB_k < \varepsilon$ then it is clair that the solution is optimal.

If the algorithm generates an infinite sequence, it suffices to show that $\lim_{k\to\infty} (UB_k - LB_k) = 0$

Let UB_q^k and LB_q^k the upper and lower bound obtained in [4] where we have shown that $\lim_{k\to\infty} (UB_q^k - LB_q^k) = 0$

i) $UB_q^k \ge UB_k$, because we add in this algorithm the pruning step and the convex/concave test which improve the upper bound.

ii) $LB_q^k \leq LB_k$ by construction.

then $0 \leq UB_k - LB_k \leq UB_q^k - LB_q^k \to 0$ when $k \to \infty$.

5 Numerical example

Example 1 $\begin{aligned} b(s) &= sins, s \in [0, 2\pi] \\ b"(s) &= -sins; -1 \leq b"(s) \leq 1; K_{\alpha} = K_q = 1, \\ LB_q(s) &= -\frac{1}{2}s(2\pi - s); LB_{\alpha}(s) = sins - \frac{1}{2}s(2\pi - s) \\ b(0) &= b(2\pi) = 0 \text{ then no pruning step.} \end{aligned}$ We solve the convex problem

$$\min\left\{z: sins - \frac{1}{2}s(2\pi - s) \le z, -\frac{1}{2}s(2\pi - s) \le z, z \in R, s \in [0, 2\pi]\right\}$$

we obtain, $z^0 = -\frac{1}{2}\pi^2, s^*_0 = \pi$ $LB_0 = z^0, UB_0 = 0$

we bisect $[0, 2\pi]$ by w – subdivision via $s_0^* = \pi$, we obtain $[0, \pi]$ and $[\pi, 2\pi]$ we begin by the interval $[0, \pi]$, we compute $K_{\alpha}^1 = 1$, $K_q^1 = 0$ Convex/concave test: $K_q^1 = 0 \Rightarrow b$ is concave on $[0, \pi]$ its minimum is attained at

0 and π We pass to the interval $[\pi, 2\pi]$, we compute $K_{\alpha}^2 = 0$, $K_q^2 = 1$ Convex/concave test: $K_{\alpha}^2 = 0 \Rightarrow b$ is convex on $[\pi, 2\pi]$ its minimum is attained at $\frac{3\pi}{2}$.

The algorithm stops at the global minimum $\overline{s}^1 = \frac{3\pi}{2}$ with $b(\frac{3\pi}{2}) = -1$

Example 2 (we take the same example 2 as in section 3) $\begin{aligned} b(s) &= sins + coss, s \in [0, 2\pi] \\ b^{"}(s) &= -sins - coss; -2 \leq b^{"}(s) \leq 2; K_{\alpha} = K_q = 2, \\ LB_q(s) &= 1 - s(2\pi - s); LB_{\alpha}(s) = sins + coss - s(2\pi - s) \\ b(0) &= b(2\pi) = 0 \text{ then no pruning step.} \end{aligned}$ We solve the convex problem

$$\min\left\{z: sins + coss - \frac{1}{2}s(2\pi - s) \le z, 1 - \frac{1}{2}s(2\pi - s) \le z, z \in \mathbb{R}, s \in [0, 2\pi]\right\}$$

we obtain, $z^0 = 1 - \pi^2, s_0^* = \pi$ $LB_0 = z^0, UB_0 = -1, \overline{s}^0 = \pi$

we bisect $[0, 2\pi]$ by w - subdivision via $s_0^* = \pi$, we obtain $[0, \pi]$ and $[\pi, 2\pi]$ we begin by the interval $[0, \pi]$, we compute $K_{\alpha}^{11} = \sqrt{2}$, $K_q^{11} = 1$ Convex/concave test: No interval discarded.

Pruning step: we compute $LB_q^{11}(s) = 1 - \frac{2s}{\pi} - \frac{1}{2}s(\pi - s) = UB_0 = -1$

we find two solutions, $\frac{1}{2}$ and π then the interval $[0, \pi]$ is reduced to the interval $[\frac{1}{2}, \pi]$ (i.e. the part $[0, \frac{1}{2}]$ is discarded).

we compute again $LB_q^{1r_11}(s)$ on the interval $[\frac{1}{2},\pi]$ and we solve the quadratic equation $LB_q^{1r_11}(s) = -1$, this procedure stops when the interval $[\frac{1}{2},\pi]$ is reduced to one point π then $UB_{11} = LB_{11} = -1$.

We pass to the second interval $[\pi, 2\pi]$, we compute $K_{\alpha}^{12} = 0$ then by the convex/concave test, b is convex on the interval $[\pi, 2\pi]$, we apply local search and find its minimum $s_{12}^* = \frac{5\pi}{4}; b(s_{12}^*) = -\sqrt{2} = UB_{12} = LB_{12}$.

We have $UB_1 = LB_1 = -\sqrt{2}$ then the algorithm stops after two iterations with the optimal solution $\overline{s}^1 = \frac{5\pi}{4}$ with $b(\frac{5\pi}{4}) = -\sqrt{2}$.

6 Conclusion

We have proposed in this theoretical paper a combination of two lower bound functions in branch and prune algorithm. the convergence is accelerated by the convex/concave test and the pruning step. The preliminary results show that this method is promising.

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