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New Underestimator for Twice Differentiable Functions with Bounded Variables

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Abstract

In this paper, a new global optimization method is proposed for an optimization problem with twice-differentiable objective function a single variable with box constraint. The method employs a difference of linear interpolant of objective and a concave function, where the former is a continuous piecewise convex quadratic function underestimator. The main objectives of this research are to determine the value of lower bound that does not need an iterative local optimizer. The proposed method is proven to have a finite convergence to locate the global optimum point. The numerical experiments indicate that the proposed method competes with another covering method.

Keywords— Global Optimization, Branch and Bound, Piecewise Convex Underestimation, Explicit Solution

Introduction

In the convex optimization, we seek a local solution widely enough to determine the optimal solution [1,2,21]. While the objective of global optimization is to find the globally best solution of possibly nonlinear models, in the possible or known presence of multiple local optima. Formally, global optimization seeks global solutions of a constrained optimization model[20]. Nonlinear models are ubiquitous in many applications,e.g., in advanced engineering design, biotechnology, data analysis, environmental management, financial planning, process control, risk management, scientific modeling, and etc. Their solution often requires a global search approach [14,19,4,23,3,22,11,18].

A variety of adaptive partition strategies have been proposed to solve global optimization models. These are based upon partition, sampling, and subsequent lower and upper bounding procedures. These operations are applied iteratively to the collection of active subsets within the feasible set. In this connection several works have been proposed among others. Adjiman et al. [5] presented the detailed implementation of the alpha BB approach and computational studies in process design problems such as heat exchanger networks, reactor-separator networks, and batch design under uncertainty.

Akrotirianakis and Floudas [7] presented computational results of the new class of convex underestimators embedded in a branch-and-bound framework for box-constrained NLPs. They also proposed a hybrid global optimization method that includes the random-linkage stochastic approach with the aim of improving the computational performance. Caratzoulas and Floudas [9] proposed novel convex underestimators for trigonometric functions.

Recently, years univariate global optimization problems have attracted common attention because they arise in many real-life applications and the obtained results can be easily generalized to the multivariate case [6,17,13,8,24,25].

In this paper, we propose an approache to find a global minimum of a univariate objective function.

In the following we will present our technique.

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A Piecewise Quadratics Underestimations ($KBBm$):

The main idea consists in constructing piecewise quadratic underestimation functions closer to the given non-convex f in a successive reduced interval $[a_k, b_k]$, and their minimums are explicitly given, Instead of using a single large square away from the objective function [16], the determination of its minimum implies a local method [5]. We propose an explicit method of quadratic relaxation of building global optimization problems with bounded variables. This construction is based on the work of authors in [16], using the quadratic splines. The generated quadratic programs have exactly explicit optimal solutions. In each interval in the target underestimated by several quadratic splines reliable to calculate the lower bounds.

The structure of the rest of the paper is as follows: Section 2 presents the two underestimators proposed in [16,5]. Section 3 discusses the construction of a new lower bound on the objective function, and describes a proposed algorithm $(KBBm)$ to solve the univariate global optimization problem with box constrained. Section 4 presents some numerical examples of different non-convex objective functions while we conclude the paper in Section 5.

Background

Consider the following global minimization problem:

$$(P)\begin{cases}\min\limits_{[a,b]} f(x) = \alpha \\ x \in X = [a,b]\end{cases},$$

with f is a non-convex twice differentiable function on X.

In what follows we give two underestimators developed by the authors, respectively in [5,16].

Underestimator in (αBB) method[5]

The underestimator in αBB method on the interval $[a, b]$ is as follows

$$L(x) = f(x) - \frac{\alpha}{2}(x - a)(b - x),$$

where $\alpha \geq \max\{0, -f(x)\}$ for all $x \in [a, b]$

This underestimator satisfies the following properties:

(1) It is convex $(i.e. LL''(x) = f''(x) + \alpha \geq 0,$ for all $x \in [a, b]$.

(2) It coincides with the function $f(x)$ at the endpoint of the interval $[a, b]$.

(3) It is an underestimator of the objective function $f(x)$.

(4) Requires solving the convex problem $minL(x);$ for all $x \in [a, b]$ to determine the values of the lower bound of the objective function $f(x)$. For more details, see [5].

Quadratic Underestimator in (KBB) Method [16].

The quadratic underestimator developed in [16] on the interval $[a, b]$ is:

$$q(x) = f(a)\frac{b-x}{b-a} + f(b)\frac{x-a}{b-a} - \frac{K}{2}(x-a)(b-x),$$

where $|f''(x)| \leq K,$ for all $x \in [a, b]$.

This quadratic underestimator satisfies the following properties:

(1) it is convex $i.e. q''(x) = K \geq 0$, for all $x \in [a, b]$.
(2) It coincides with the function $f(x)$ at the endpoint of the interval $[a, b]$.
(3) It is an underestimator of the objective function $f(x)$.
(4) The values of the lower bound are given explicitly. For more details, see [16].

Advantages and disadvantages of two methods.

(1) The advantage of (αBB), is the best initial lower bound obtained, also the underestimator is close to the objective function (see Table 2,3).
(2) The disadvantage of (αBB), uses a local method for determining the values of the lower bounds.
(3) The advantage of (KBB), is the values of the lower bounds are given explicitly.
(4) The disadvantage of (KBB), is the initial lower bound is very far from the optimal solution, also the underestimator is far away from objective function (see Table 2,3).

The Proposed Underestimator(KBBm)

In this section we present the new lower bound. In this lower bound we merge the advantages of KBB and αBB.

Let $X = [a, b]$ be a bounded closed interval in R . Let f be a continuously twice differentiable function on X. Let x^0 and x^1 be two real numbers in $[a, b]$ such that $x^0 \leq x^1$. Let l_0 and l_1 be real valued functions defined by

$$l_0(x) = \frac{x^0 - x}{x^1 - x^0} \text{ if } x^0 \leq x \leq x^1, \; l_1(x) = \frac{x - x^0}{x^1 - x^0} \text{ if } x^0 \leq x \leq x^1.$$

For all x in the interval [x^0, x^1], we have $l_0(x) + l_1(x) = 1$. We have also $l_i(x^j)$ is equal to 0 if $i \neq j$; and 1 otherwise. Let $h = x^1 - x^0$ and $L_h f$ be the piecewise linear interpolant to f at points x^0, x^1 see [10, 12]. Such that

$$L_h f(x) = \sum_{i=0}^{1} l_i(x) f(x^i).$$

Knowing that $f(x)$ is a univariate function that needs to be underestimated in the interval $[a, b]$. Suppose that the nodes are chosen to be equally spaced in $[a, b]$, so that

$$x_i = a + ih, h = \frac{b - a}{n}, i = 0, \ldots, n.$$

For every interval $[x_i, x_{i+1}]$ we construct the corresponding local quadratic underestimator as follows

$$p_i(x) = L_h f(x) - Q_i(x),$$

where

$$Q_i(x) = {}^1/_2 K_i (x - x_i)(x_{i+1} - x),$$

Figure 1.Show the tightness of our underestimator $p(x)$ than the $q(x)$ for $n = 2$

where K_i is an upper bound of the second derivative which is valid for $[x_i, x_{i+1}]$. Instead of considering one quadratic lower bound over $[a, b]$, we construct a piecewise quadratic lower bound.

In the following theorem we will show that the new lower bound is tighter than the lower bound constructed in [16].

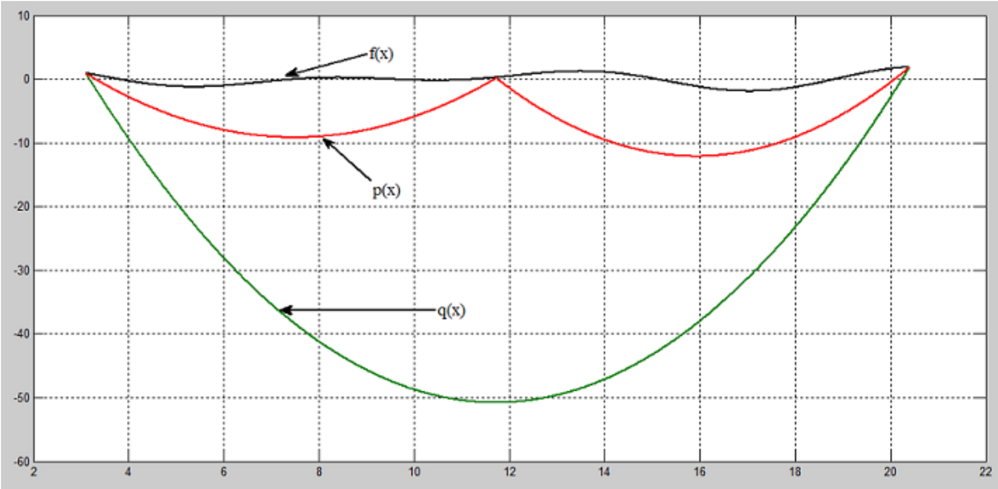
Theorem We have

$$q(x) \leq p(x) \leq f(x), \qquad \forall x \in [a, b],$$

where

$p(x) = p_i(x);\ \forall x \in [x_i, x_{i+1}];\ i = 0, \ldots n-1.$

The function $p(x)$ *is a piecewise convex valid underestimator of* $f(x)$ *for all* x *in* $[a, b]$, *and it is tighter than the underestimator* $q(x)$ *introduced in [16].*



In each sub-interval $[x_i, x_{i+1}]$, one have to compute a quadratic lower bound underestimation of the objective function f.

$$x_i^* = \begin{cases} \frac{1}{2}(x_i + x_{i+1}) - \frac{1}{K_i}\frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} & if\ x \in [x_i, x_{i+1}] \\ x_i & if\quad x \le x_i \\ x_{i+1} & if\ x \ge x_{i+1} \end{cases} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (*)$$

Now, we compute the values of $p_i(x_i^*)$ in order to detect the best lower bound we compare all lower bounds and preserve the smallest one as follows:

$$LB^k = min p_i(x_i^*).$$

The upper bound is calculated by the following comparisons and maintains the best ever. The objective function is evaluated at different points so has to determine the upper bound.

$$UB^k = min\{min f(x_i^*), min f(x_i)\}.$$

Remark . The proposed underestimator $KBBm$ verifies the following properties.

(1) It is piecewise convex on $[a, b]$.
(2) It coincides with the function $f(x)$ at the endpoint of the interval $[x_i, x_{i+1}]$ for all $i = 0, \ldots, n-1$.
(3) It is an underestimator of the objective function $f(x)$.
(4) The values of the lower bound are given explicitly.
(5) When we double the quadratic we obtained a good lower bounds see Table (5).

The different steps for solving the problem (P) are summarized in the following proposed algorithm:

Algorithm
Input :

- $[a, b]$: A real interval.
- ε:The accuracy.
- f: The objective function.
- n: The number of quadratic.

Output :

- x^*: The global minimum of f.

(1) Initialization step $k = 0$
(a) for all $i = 0, \dots, n$ Compute $x_i = a + \frac{b-a}{n} i$, and set $M = \coprod_{i=0}^{n-1}\{[x_i, x_{i+1}]\}$
(b) Compute K_i such that $|f''(x)| \leq K_i$ on each $[x_i, x_{i+1}]$ for all $i = 0, \dots, n-1$
(c) Compute x_i^* by using (*) for all $i = 0, \dots, n-1$
(d) Compute $UB^k = min\{minf(x_i^*), minf(x_i)\}$
(e) Set $LB^k = minLB_i^k$ with $LB_i^k = p_i(x_i^*)$
(f) $\bar{\imath}$ is the index corresponding to $minLB_i^k$
(2) Iteration step
While $(UB^k - LBk > \varepsilon$ and $M \neq \emptyset)$ do
(a) $a := x_{\bar{\imath}},\ b := x_{\overline{i+1}}$ and apply step a,b,c,and d
(b) Update UB^k
(c) For all $i = 1, \dots, m;\ (m = card\ (M))$

- Elimination step : if $(UB^k - LB_i^k < \varepsilon)$ then remove $[x_i, x_{i+1}]$ from M
- Selection step : if $(UB^k - LB_i^k \geq \varepsilon)$ then $minLB_i^k$, $\bar{\imath}$ is the index corresponding to $minLB_i^k$

(d) $k = k + 1$
end While

(3) $x^* = x^k$ is the optimal solution corresponding to the best UB^k found.
end algorithm

Theorem. [Convergence of the algorithm]

Either the algorithm is infinite or it generates a bounded sequence $\{x_k\}$. Any accumulation point of the sequence is a global optimal solution of (P). We have: $UB^k \downarrow \alpha,\ \ LB^k \uparrow \alpha$.

Computational Aspects and Results

To measure the performances of our $KBBm$ algorithm, we perform a comparative study with KBB and αBB. These algorithms are implemented in C programming language with double precision floating point, and run on a computer with an Intel (R) core (TM) i3-311MCP4 with CPU 2.40GHz. Numerical tests are performed in two parts on a set of test functions. In the first experiment, we compare the performances of the KBB, αBB and the $KBBm$ algorithms on a set of 10 functions. Here, we include a method that computes the positive numbers α and K [15]. The number of the quadratic functions used in $KBBm$ at each iteration as fixed to $n = 16$. And the accuracy fixed to $\varepsilon = 10^{-6}$. In the second experiment we were tested the $KBBm$ algorithm according to the initial lower bound obtained for different numbers of quadratic function used on a set of 20 functions.

In our results, we consider the following notations as table anterior :

- f^* is the optimum obtained

- LB_0 is the initial lower bound
- T_{CPU} is the execution time in seconds
- m is the total number of interval
- m_e is the number of intervals eliminated
- LM is the number of local minimum
- GM is the number of global minimum
- * An asterisk denotes that the lower bond is equal to the known global optimum f^*, within six decimal digits of accuracy.

Table 1:
Test Functions

Exp	$f(x)$	$[x^L, x^U]$	LM	GM	opt
1	$e^{-3x} - \sin^3 x$	$[0, 20]$	4	1	-1
2	$\cos x - \sin(5x) + 1$	$[0.2, 7]$	6	1	-0.952897
3	$x + \sin(5x)$	$[0.2, 7]$	7	1	-0.077590
4	$e^{-x} - \sin(2\pi x)$	$[0.2, 7]$	7	1	-0.478362
5	$\ln(3x)\ln(2x) - 0.1$	$[0.2, 7]$	1	1	-0.141100
6	$\sqrt{x}\sin^2 x$	$[0.2, 7]$	3	2	0
7	$2\sin x e^{-x}$	$[0.2, 7]$	2	1	-0.027864
8	$2\cos x + \cos(2x) + 5$	$[0.2, 7]$	3	2	3.5
9	$\sin x$	$[0, 20]$	4	3	-1
10	$\sin x \cos x - 1.5\sin^2 x + 1.2$	$[0.2, 7]$	3	2	-0.451388
11	$(x - x^2)^2 + (x-1)^2$	$[-10, 10]$	1	1	0
12	$\frac{x^2}{20} - \cos x + 2$	$[-20, 20]$	7	1	1
13	$x^2 - \cos(18x)$	$[-5, 5]$	29	1	-1
14	e^{x^2}	$[-10, 10]$	1	1	1
15	$(x + \sin x)\, e^{-x^2}$	$[-10, 10]$	1	1	-0.824239
16	$x^4 - 12x^3 + 47x^2 - 60x - 20e^{-x}$	$[-1, 7]$	1	1	-32.78126
17	$x^6 - 15x^4 + 27x^2 + 250$	$[-4, 4]$	2	2	7
18	$x^4 - 10x^3 + 35x^2 - 50x + 24$	$[-10, 20]$	2	2	-1
19	$24x^4 - 142x^3 + 303x^2 - 276x + 3$	$[0, 3]$	2	1	-89
20	$\cos x + 2\cos(2x)\, e^{-x}$	$[0.2, 7]$	2	1	-0.918397

Table 2:
Computation Results for 10 Functions for αBBAlgorithm

Exp		αBB			
	T_{cpu}	m	m_e	LB_0	f^*
1	0	47	24	-273.76041	-0.99999
2	0	17	9	-65.9109	-0.95203
3	0	31	16	-118.96147	-0.07759
4	0	15	8	-121.60896	-0.47797
5	0	11	6	-527.67986	-0.14099
6	0	13	7	-2733.29510	0.00199
7	0	13	7	-18.57601	-0.02761
8	0	11	6	-28.84495	3.56245
9	0	13	7	-46.40909	-0.99997
10	0	17	9	-29.62761	-0.45138

Table 3:
Computation Results for 10 Functions for KBB Algorithm

Exp		KBB			
	T_{cpu}	m	m_e	LB_0	f^*
1	2.211	55	28	-564.01754	-1
2	10.645	25	13	-116.08120	-0.95289
3	4.604	25	13	-117.80163	-0.07758
4	3.576	57	29	-121.20354	-0.47834
5	3.312	19	10	-528.13263	-0.14110
6	2.854	29	15	-6664.14641	0
7	3.132	67	34	-5.50269	-0.02786
8	3.012	21	11	-14.03655	3.5
9	2.293	15	8	-45.19193	-1
10	3.460	27	14	-29.66644	-0.45139

The execution time required to achieve the optimal value is considered as a reliable criterion to the algorithm's performances. According to the numerical results summarized, in Table (3) and Table (4), the performances of the proposed method are clearly better than the performance of the KBB method. As the best initial lower bound obtained remains an important criterion for measuring the validity of the underestimator. In Table (2), Table (3) and Table (4), the comparative study of the quality of the initial lower bound found by the three algorithms show that our method is better than the two methods. In Table 5 just confirmed the competence of our method by doubling the number of quadratic we can notice that the values of the lower bound are improved.

Table 4:
Computation Results for 10 Functions for KBB_m Algorithm with n=16

Exp	KBB_m				
	T_{cpu}	m	m_e	LB_0	f^*
1	0	144	136	−2.26691	−1
2	0	32	31	−0.97784	−0.9529
3	0	48	46	−0.09467	−0.07759
4	0	176	166	−0.65053	−0.47820
5	0	48	46	−1.73375	−0.14110
6	0	48	46	−0.23383	0
7	0	112	106	−0.04618	−0.02786
8	0	48	46	3.49276	3.50001
9	0	64	61	−1.00563	−1
10	0	64	61	−0.45957	−0.45139

Table 5:
LB_0 values obtained by $KBBm$

n	2	4	8	16	32	64	128
1	−152.72	−45.16	−7.15	−2.26	*	*	*
2	−28.43	−7.92	−2.16	−0.97	*	*	*
3	−28.45	−6.17	−1.34	−0.094	*	*	*
4	−30.018	−8.85	−2.207	−0.65	−0.49	*	*
5	−121.3	−29.66	−7.17	−1.73	−0.40	−0.149	−0.1417
6	−448.19	−41.56	−3.542	−0.23	−0.0019	−0.0002	−0.00003
7	−1.307	−0.340	−0.104	−0.04	−0.03	−0.02	−0.028
8	0.33	2.54	3.394	3.49	*	*	*
9	−11.23	−3.751	−1.141	−1.005	*	*	*
10	−5.85	−1.98	−0.598	−0.459	−0.453	−0.452	−0.4515
11	−16118.1	−1297.05	−107.4	−9.34	−0.67	−0.09	−0.01113
12	1	*	*	*	*	*	*
13	−20.42	−2.2	*	*	*	*	*
14	*	*	*	*	*	*	*
15	−173493.6	−27703.7	−7855.9	−769.2	−575.3	−48.21	−46.4
16	−19351.54	−576.321	−45.152	−33.67	−32.84	−32.80	−32.789
17	−14875.91	−2957.18	−362.63	−21.88	4.71	6.82	6.98
18	−93572.1	−9016.69	−1032.09	−142.7	−27.31	−7.07	−2.4
19	−578.6	−141.98	−95.79	−89.8	−89.1	−89.01	−89.001
20	−6.906	−2.59	*	*	*	*	*

Conclusion

We presented a method of underestimation of non-convex objective based on piecewise quadratic functions have explicit minimums. A comparison of the lower bounds favors such quadratic against other guaranteeing the underestimation of the objective. This approach is validated by considering a deterministic branch and bound which is fully detailed and allows certifying still coaching the value of the global minimum at the end of the performance. Many digital experiences are performed, that confirm the effectiveness of this new acceleration technique. The performance of the proposed procedure depends on the quality of the chosen lower bound of f. Such that, our piecewise quadratic lower bounding functions is better than two underestimators introduced in [16, 5].

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