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# TIGHTER CONVEX UNDERESTIMATOR FOR GENERAL TWICE DIFFERENTIABLE FUNCTION FOR GLOBAL OPTIMIZATION

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**Abstract.** This paper proposes a new convex underestimator for general $C^2$ nonconvex functions. The new underestimator can be used in the branch and bound algorithm $\alpha$BB for solving global optimization problems. We show that the new underestimator is tighter than the classical underestimator in the $\alpha$BB method.

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## 1. Introduction

We consider the following problem:

$$(P)\begin{cases} \min f(x) \\ x \in [X^L, X^U] \subset \mathbb{R}^n \end{cases}$$

where $f$ is a nonconvex and $C^2$-continuous function on the box $[X^L, X^U]$. Due to the nonconvex function $f$, the problem (P) may posses more than one local minimum, therefore (P) is a global optimization problem. In last decades, several methods have been studied in the literature for global optimization problems. We can mention deterministic approaches methods for example interval analysis [8,9], DC programming [4] and branch and bound methods [5,13].

The deterministic approach developed in [14] is based on a combination of the DC (Difference of Convex functions) programming and a Branch and Bound algorithm for solving binary quadratic programs (BQP) which is a global optimization problem. The authors in [14] reformulate the (BQP) as a DC program by using an exact penalty, in order to apply the DC algorithm.

The $\alpha$BB method developed in [5], consists of constructing a convex underestimator and using it in a branch and bound algorithm to generate two sequences of lower and upper bounds which converge to an optimal solution.

A refinement of the classical $\alpha$BB convex underestimator based on piecewise quadratic perturbation functions is developed in [11]. Another class of $\alpha$BB convex underestimator based on a nonlinear concave relaxation, is developed in [3]. The authors in [13], developed a quadratic convex underestimator and used a branch and bound algorithm for solving global optimization problems.

*Keywords.* Convex underestimator, global optimization, $\alpha$BB method.

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The quality of the optimal solution depends on the tightness of the underestimator, where the tighter underestimator decreases the separation distance between the upper bound of the nonconvex function and its convex underestimator, which increases the efficiency of the convergence of the global optimization algorithm. Since the tightness of the underestimator is extremely important, therefore in [1, 12] the researchers have developed methods based on interval analysis to improve lower bounds on eigenvalues which is the key of the tightness underestimator.

The main goal of our paper is to develop a new convex underestimator which is tighter than the classical $\alpha$BB underestimator developed in [5].

The structure of the paper is as follows. The two underestimators developed in [5, 13] with their properties are presented in Section 2. In Section 3, the new relaxation and underestimator are stated with their properties. Computational results are presented in Section 4.

## 2. Convex underestimator functions in $\mathbb{R}^n$

### 2.1. Quadratic convex underestimator [13]

The quadratic convex underestimator on $\left[X^L, X^U\right]$ is developed in [13] as follows:

$$LB_q(x) = Lh(x) - \frac{K_q}{2}\sum_{i=1}^{n}\left(x_i^U - x_i\right)\left(x_i - x_i^L\right) \tag{1}$$

where $K_q \geq \|H_f\|$, $Lh(x)$ is the linear interpolant of $f$, with $H_f$ the hessian matrix of $f(x)$ on $\left[X^L, X^U\right]$. Let a symetric matrix $A = (a_{ij})$, then the norm $\|A\|$ used in this paper is defined as follows: $\|A\| = \max_{i=1,\ldots,n}\sum_{j=1}^{n}|a_{ij}|$.

This quadratic underestimator have the following properties:

(1) $LB_q(x)$ coincides with $f(x)$ at the endpoints of $\left[X^L, X^U\right]$.
(2) $LB_q(x)$ is a convex function on $\left[X^L, X^U\right]$.
(3) $LB_q(x)$ is an underestimator of $f(x)$ on $\left[X^L, X^U\right]$.

For more details see [13].

### 2.2. $\alpha$BB Convex underestimator [5]

The $\alpha$BB convex underestimator on $\left[X^L, X^U\right]$ is developed as follows:

$$LB_\alpha(x) = f(x) - \sum_{i=1}^{n}\frac{\alpha_i}{2}\left(x_i^U - x_i\right)\left(x_i - x_i^L\right), \tag{2}$$

with $\alpha_i \geq \max\{0, -\min\lambda_i(x)\}$, where $\lambda_i(x)$ is the $i$th eigenvalue of the hessian matrix $H_f$ on $\left[X^L, X^U\right]$. However, it is very difficult to calculate the minimum eigenvalue of the hessian matrix for an arbitrary nonconvex function on the box $\left[X^L, X^U\right]$, therefore one of the most used methods to compute efficient values of $\alpha_i$, is the scaled Gershgorin in [2] defined as follows:

$$\alpha_i = \max\left\{0, -\left(\underline{f_{ii}} - \sum_{i\neq j}\left\{|\underline{f_{ij}}|, |\overline{f_{ij}}|\right\}\frac{d_j}{d_i}\right)\right\}, \quad i = 1, \ldots, n \tag{3}$$

where $\underline{f_{ij}}$ and $\overline{f_{ij}}$ are the lower and upper bounds of $\frac{\partial^2 f}{\partial x_i \partial x_j}$ from the hessian matrix $H_f$ which are computed by the interval analysis technique where $d_i = x_i^U - x_i^L$ is a choice of $d_i$ given in [2] which means that variables with a wide range have a larger effect on the quality of the underestimator than variables with a smaller range.

The $\alpha$BB underestimator have the following properties:

(1) $LB_\alpha(x)$ coincides with $f(x)$ at the endpoints of $\left[X^L, X^U\right]$.
(2) $LB_\alpha(x)$ is a convex function on $\left[X^L, X^U\right]$.
(3) $LB_\alpha(x)$ is an underestimator of $f(x)$ on $\left[X^L, X^U\right]$.

For more details see [5].

## 3. New convex underestimator function

### 3.1. New concave relaxation

We first present a new relaxation as follows:

$$\phi(x;\sigma) = \sum_{i=1}^{n} \sigma_i \left( \frac{\ln\left(\frac{x_i - x_i^L}{x_i^U - x_i^L} + 1\right) + \ln\left(\frac{x_i^U - x_i}{x_i^U - x_i^L} + 1\right)}{\ln(2)} - 1 \right) \tag{4}$$

with $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n)$ where $\sigma_i$ is a non negative parameter and has a role from the nonconvex twice differentiable function $f(x)$, to construct a tighter convex underestimator.

**Proposition 1.** $\phi(x;\sigma) = 0$ *at the endpoints of the interval* $\left[X^L, X^U\right]$.

*Proof.* Let $x^c = (x_1^c, x_2^c, \ldots, x_n^c)$ be an endpoint of the interval $\left[X^L, X^U\right]$, where $x_i^c = x_i^L$ or $x_i^c = x_i^U$. Then we have

$$\ln\left(\frac{x_i - x_i^L}{x_i^U - x_i^L} + 1\right) = 0 \quad \text{and} \quad \ln\left(\frac{x_i^U - x_i}{x_i^U - x_i^L} + 1\right) = \ln(2),$$

or

$$\ln\left(\frac{x_i - x_i^L}{x_i^U - x_i^L} + 1\right) = \ln(2) \quad \text{and} \quad \ln\left(\frac{x_i^U - x_i}{x_i^U - x_i^L} + 1\right) = 0.$$

So, we have $\phi(x^c;\sigma) = 0$. □

**Proposition 2.** $\phi(x;\sigma)$ *is a concave function over the interval* $\left[X^L, X^U\right]$.

*Proof.* The hessian matrix of $\phi(x;\sigma)$ is $H\phi(x;\sigma)$, where $H\phi$ is a diagonal matrix and for each diagonal element we have

$$h\phi_{ii} = \sigma_i \left( -\frac{1}{(x_i^U - x_i^L)^2 \left(\frac{x_i - x_i^L}{x_i^U - x_i^L} + 1\right)^2} - \frac{1}{(x_i^U - x_i^L)^2 \left(\frac{x_i^U - x_i}{x_i^U - x_i^L} + 1\right)^2} \right) \frac{1}{\ln(2)}.$$

Since $\sigma_i \geq 0$ and $\ln(2) \geq 0$, then $h\phi_{ii} \leq 0$, $\forall x_i \in \left[x_i^L, x_i^U\right]$ for $i = 1, \ldots, n$. Therefore, the matrix $H\phi(x;\sigma)$ is negative semi-definite. Hence, $\phi(x;\sigma)$ is a concave function. □

**Proposition 3.** $\phi(x;\sigma) \geq 0$, *for all* $x \in \left[X^L, X^U\right]$.

*Proof.* From the above propositions we have $\phi(x;\sigma)$ is a concave function and $\phi(x;\sigma) = 0$ at the endpoints of the interval $\left[X^L, X^U\right]$. Hence, $\phi(x;\sigma) \geq 0$, for all $x \in \left[X^L, X^U\right]$. □

**Proposition 4.** $H\phi(x;\sigma)$ *is the hessian matrix of* $\phi(x;\sigma)$, *each element* $h\phi_{ii}$ *of* $H\phi(x;\sigma)$ *is a concave function and achieves its maximum at the middle point and its minimum at the endpoints of* $\left[X^L, X^U\right]$.

*Proof.* From the hessian matrix $H\phi(x;\sigma)$ we have

$$h\phi_{ii} = \sigma_i \left( -\frac{1}{\left(x_i^U - x_i^L\right)^2 \left(\frac{x_i - x_i^L}{x_i^U - x_i^L} + 1\right)^2} - \frac{1}{\left(x_i^U - x_i^L\right)^2 \left(\frac{x_i^U - x_i}{x_i^U - x_i^L} + 1\right)^2} \right) \frac{1}{\ln(2)}.$$

The second derivative of $H\phi(x;\sigma)$ is

$$\frac{\partial^2}{\partial x_i^2} H\phi(x;\sigma) = \frac{\sigma_i}{\ln(2)\left(x_i^U - x_i^L\right)^2} \left( -\frac{6}{\left(x_i^U - x_i^L\right)^2 \left(\frac{x_i - x_i^L}{x_i^U - x_i^L} + 1\right)^4} - \frac{6}{\left(x_i^U - x_i^L\right)^2 \left(\frac{x_i^U - x}{x_i^U - x_i^L} + 1\right)^4} \right).$$

It's clear that $\frac{\partial^2}{\partial x_i^2} H\phi(x;\sigma) \leq 0$, $\forall x_i \in \left[x_i^L, x_i^U\right]$. Hence, $h\phi_{ii}$ is a concave function and we have also

$$\frac{\partial}{\partial x_i} H\phi(x;\sigma) = \frac{\sigma_i}{\ln(2)\left(x_i^U - x_i^L\right)^2} \left( \frac{2}{\left(x_i^U - x_i^L\right) \left(\frac{x_i - x_i^L}{x_i^U - x_i^L} + 1\right)^3} - \frac{2}{\left(x_i^U - x_i^L\right) \left(\frac{x_i^U - x_i}{x_i^U - x_i^L} + 1\right)^3} \right).$$

$\frac{\partial}{\partial x_i} H\phi(x;\sigma) = 0$ at the middle point: $x_i^{mid} = \frac{x_i^U + x_i^L}{2}$.

Furthermore, since $h\phi_{ii}$ is a concave function, then it achieves its minimum at the endpoints of $\left[x_i^L, x_i^U\right]$. So, we have

$$\min h\phi_{ii} = h\phi_{ii}\left(x_i^L;\sigma\right) = h\phi_{ii}\left(x_i^U;\sigma\right) = \sigma_i \left( \frac{-\frac{1}{\left(x_i^U - x_i^L\right)^2 2^2} - \frac{1}{\left(x_i^U - x_i^L\right)^2}}{\ln(2)} \right). \tag{5}$$

□

### 3.2. New convex underestimator

Now, we present our new convex underestimator on $\left[X^L, X^U\right]$ as follows:

$$LB(x) = f(x) - \phi(x;\sigma). \tag{6}$$

**Proposition 5.** *$LB(x)$ coincides with $f(x)$ at the end points of $\left[X^L, X^U\right]$.*

*Proof.* We have $x^c = (x_1^c, x_2^c, \ldots, x_n^c)$ a vertex point of $\left[X^L, X^U\right]$, where $x_i^c = x_i^L$ or $x_i^c = x_i^U$. We know from Proposition 1 that $\phi(x^c;\sigma) = 0$.

Hence, $LB(x^c) = f(x^c)$. □

**Proposition 6.** $LB(x) \leq f(x), \quad \forall x \in \left[X^L, X^U\right]$.

*Proof.* We have proved in Proposition 3, that $\phi(x;\sigma) \geq 0$. Therefore,

$LB(x) = f(x) - \phi(x;\sigma) \leq f(x), \quad \forall x \in \left[X^L, X^U\right]$. □

**Proposition 7.** *The maximum separation distance between $f(x)$ and $LB(x)$ is reached at the middle point $x^{mid} = \frac{x^L + x^U}{2}$ of the interval $\left[X^L, X^U\right]$.*

*Proof.* We have
$$\max_{x\in[X^L,X^U]} f(x) - LB(x) = \max_{x\in[X^L,X^U]} \phi(x;\sigma). \tag{7}$$
We know that $\phi(x;\sigma)$ is a concave function. Furthermore, the first derivative of $\phi(x;\sigma)$ is
$$\frac{\partial}{\partial x_i}\phi(x;\sigma) = \sigma_i \left( \frac{\dfrac{1}{\left(x_i^U - x_i^L\right)\left(\dfrac{x_i - x_i^L}{x_i^U - x_i^L} + 1\right)} - \dfrac{1}{\left(x_i^U - x_i^L\right)\left(\dfrac{x_i^U - x_i}{x_i^U - x_i^L} + 1\right)}}{\ln(2)} \right). \tag{8}$$
Therefore, $\frac{\partial}{\partial x_i}\phi(x;\sigma) = 0$ at the middle point $x_i^{mid} = \frac{x_i^L + x_i^U}{2}$. Hence,
$$\max_{x\in[X^L,X^U]} \phi(x;\sigma) = \phi\left(x^{mid};\sigma\right) = \sum_{i=1}^{n} \sigma_i \left( \frac{2\ln\left(\dfrac{3}{2}\right)}{\ln(2)} - 1 \right). \tag{9}$$
□

From the above proposition, we notice that the maximum separation distance between the new underestimator and the original function, depends on $\sigma$. Moreover, in the following proposition we will show that $\sigma$ depends on the interval $\left[X^L, X^U\right]$.

**Proposition 8.** *Let the intervals $X = \left[X^L, X^U\right]$ and $Y = \left[Y^L, Y^U\right]$, where $X \subseteq Y \subseteq \mathbb{R}^n$. Then, the underestimator $LB_X(x) = f(x) - \phi(x;\sigma)$, $\forall x \in X$ is tighter than the underestimator $LB_Y(x) = f(x) - \phi(y;\sigma)$, $\forall y \in Y$.*

*Proof.* Since $X \subseteq Y$, then for every $i = 1, \ldots, n$, we have
$$x_i^U \le y_i^U \quad \text{and} \quad x_i^L \ge y_i^L,$$
then
$$x_i^U - x_i^L \le y_i^U - y_i^L,$$
with
$$x_i - x_i^L \le y_i - y_i^L \quad \text{and} \quad x_i^U - x_i \le y_i^U - y_i.$$
The logarithm function is monotonically increasing and from the above three inequalities, we have
$$\left(\frac{x_i - x_i^L}{x_i^U - x_i^L} + 1\right) \le \left(\frac{y_i - y_i^L}{y_i^U - y_i^L} + 1\right) \Leftrightarrow \ln\left(\frac{x_i - x_i^L}{x_i^U - x_i^L} + 1\right) \le \ln\left(\frac{y_i - y_i^L}{y_i^U - y_i^L} + 1\right),$$
and
$$\left(\frac{x_i^U - x_i}{x_i^U - x_i^L} + 1\right) \le \left(\frac{y_i^U - y_i}{y_i^U - y_i^L} + 1\right) \Leftrightarrow \ln\left(\frac{x_i^U - x_i}{x_i^U - x_i^L} + 1\right) \le \ln\left(\frac{y_i^U - y_i}{y_i^U - y_i^L} + 1\right).$$
Therefore,
$$\ln\left(\frac{x_i - x_i^L}{x_i^U - x_i^L} + 1\right) + \ln\left(\frac{x_i^U - x_i}{x_i^U - x_i^L} + 1\right) \le \ln\left(\frac{y_i - y_i^L}{y_i^U - y_i^L} + 1\right) + \ln\left(\frac{y_i^U - y_i}{y_i^U - y_i^L} + 1\right).$$

Now, since it is known that $\sigma_i \geq 0, \forall i = 1, \dots, n$, we can construct the two different underestimators as follows:

$$-\sigma_i \left( \frac{\ln\left(\frac{x_i - x_i^L}{x_i^U - x_i^L} + 1\right) + \ln\left(\frac{x_i^U - x_i}{x_i^U - x_i^L} + 1\right)}{\ln(2)} - 1 \right) \geq -\sigma_i \left( \frac{\ln\left(\frac{y_i - y_i^L}{y_i^U - y_i^L} + 1\right) + \ln\left(\frac{y_i^U - y_i}{y_i^U - y_i^L} + 1\right)}{\ln(2)} - 1 \right).$$

So, $LB_X(x) \geq LB_Y(x)$. □

It is known that during the execution of the $\alpha$BB algorithm, the box constrained of each sub-domain is different, so we adapt the lower bound to each sub-domain. In fact, the above proposition shows that for each time the domain is split into sub-domains, the proposed underestimator produces tighter lower bound at each subdomain. Therefore, the sequence of these lower bounds converges to a global optimal solution.

In the following, we show that the new underestimator can be convex with an initial value of $\sigma_i$, and with that value, the new underestimator is tighter than the underestimator presented in $\alpha$BB method. Furthermore, an algorithm presented in [3] is used to guarantee the convexity of our new underestimator.

We can start by initializing the values of $\sigma_i$ by solving the following equation:

$$\gamma_i + \sigma_i \left( \frac{\frac{1}{\left(x_i^U - x_i^L\right)^2 2^2} + \frac{1}{\left(x_i^U - x_i^L\right)^2}}{\ln(2)} \right) = 0 \tag{10}$$

where $\gamma_i \leq 0$, are the nonconvexities values of the original twice differentiable function. Therefore, the initial values of the parameter $\sigma_i$ from equation (10) can guarantee the convexity of our new underestimator on $\left[X^L, X^U\right]$. The values of $\gamma_i$ are computed by using the scaled Gerschgorin method [2] as follow:

$$\gamma_i = -\max\left\{0, -\left(\underline{f_{ii}} - \sum_{i \neq j} \left\{|\underline{f_{ij}}|, |\overline{f_{ij}}|\right\} \frac{d_j}{d_i}\right)\right\}, \quad i = 1, 2 \dots, n. \tag{11}$$

We can notice that : $\gamma_i = -\alpha_i$, $i = 1, 2 \dots, n$.

**Theorem 9.** *There exist $\gamma = (\gamma_1, \gamma_2 \dots, \gamma_n)$ such that, if $\sigma = (\sigma_1, \sigma_2 \dots, \sigma_n)$ is the solution of the equation (10), then $LB(x)$ is convex.*

*Proof.* First, we need to know that: $-\sigma_i \left( \frac{\frac{1}{(x_i^U - x_i^L)^2 2^2} + \frac{1}{(x_i^U - x_i^L)^2}}{\ln(2)} \right)$ is monotonically decreasing, for that we assume that: $0 \leq \sigma_i' \leq \sigma_i''$. Then, we have

$$-\sigma_i' \left( \frac{\frac{1}{\left(x_i^U - x_i^L\right)^2 2^2} + \frac{1}{\left(x_i^U - x_i^L\right)^2}}{\ln(2)} \right) \geq -\sigma_i'' \left( \frac{\frac{1}{\left(x_i^U - x_i^L\right)^2 2^2} + \frac{1}{\left(x_i^U - x_i^L\right)^2}}{\ln(2)} \right).$$

Hence, $-\sigma_i \left( \frac{\frac{1}{(x_i^U - x_i^L)^2 2^2} + \frac{1}{(x_i^U - x_i^L)^2}}{\ln(2)} \right)$ is monotonically decreasing and it goes to $-\infty$ when $\sigma_i \longmapsto +\infty$.

We already know from the hessian matrix of $f(x)$, that $\frac{\partial^2 f(x)}{\partial x_i \partial x_j}$ is bounded on the interval $\left[X^L, X^U\right]$. Therefore, there exist $\gamma_i < 0$, such that the parameter $\sigma_i$ which is the solution of equation (10) and from (5), can make $\frac{\partial^2 \phi(x;\sigma)}{\partial x_i^2}$ the dominant element in the $i$th row of the hessian matrix $HLB(x)$. Hence, $LB(x)$ is a convex function. □

**Theorem 10.** *$LB(x) \geq LB_\alpha(x)$ on the interval $\left[X^L, X^U\right]$.*

*Proof.* We have

$$LB(x) - LB_\alpha(x) = -\sum_{i=1}^{n} \sigma_i \left( \frac{\ln\left(\frac{x_i - x_i^L}{x_i^U - x_i^L} + 1\right) + \ln\left(\frac{x_i^U - x_i}{x_i^U - x_i^L} + 1\right)}{\ln(2)} - 1 \right) + \sum_{i=1}^{n} \frac{\alpha_i}{2} \left(x_i^U - x_i\right)\left(x_i - x_i^L\right).$$

If we use the hessian matrix $H\left(LB(x) - LB_\alpha(x)\right)$, then its $i$th diagonal element is

$$\sigma_i \left( \frac{1}{\left(x_i^U - x_i^L\right)^2 \left(\frac{x_i - x_i^L}{x_i^U - x_i^L} + 1\right)^2} + \frac{1}{\left(x_i^U - x_i^L\right)^2 \left(\frac{x_i^U - x_i}{x_i^U - x_i^L} + 1\right)^2} \right) \frac{1}{\ln(2)} - \alpha_i.$$

Now, we combine the results from Proposition 4, $\sigma_i$ the solution of equation (10) and the equation (11), to obtain the following result:

$$H\left(LB(x) - LB_\alpha(x)\right) \leq \sigma_i \left( \frac{\frac{1}{\left(x_i^U - x_i^L\right)^2 2^2} + \frac{1}{\left(x_i^U - x_i^L\right)^2}}{\ln(2)} \right) - \alpha_i = 0. \tag{12}$$

Therefore, $LB(x) - LB_\alpha(x)$ is a concave function, moreover $LB(x)$ coincides with $LB_\alpha(x)$ at the endpoints of the interval $\left[X^L, X^U\right]$. Hence, $LB(x) \geq LB_\alpha(x)$. □

An algorithm described in [3] can be used on $\sigma_i$ values to guarantee that the new underestimator is convex and tighter than the $\alpha$BB underestimator, for that, the following theorems show the relationship between the maximum separation distance of $LB(x)$ and $LB_\alpha(x)$ from the original function $f(x)$ on the interval $\left[X^L, X^U\right]$ for certain values of the parameters $\sigma$ and $\alpha$.

**Theorem 11.** *Let $\underline{\sigma} = (\underline{\sigma_1}, \ldots, \underline{\sigma_n})$ the solution of (10), then for $\underline{\alpha} = (\underline{\alpha_1}, \ldots, \underline{\alpha_n})$ where*

$$\underline{\alpha_i} = \left(\frac{8\underline{\sigma_i}}{(x^U - x^L)^2}\right)\left(\frac{2\ln\left(\frac{3}{2}\right)}{\ln(2)} - 1\right), \quad \text{for} \quad i = 1, 2 \ldots, n, \tag{13}$$

*$LB(x)$ and $LB_\alpha(x)$ have the same maximum separation distance between them and the function $f(x)$ for $\underline{\sigma}$ and $\underline{\alpha}$.*

*Proof.* The maximum separation distance between $LB_\alpha(x)$ and $f(x)$ is given by

$$d_{\alpha BB}^{\max}(\alpha) = \sum_{i=1}^{n} \frac{\alpha_i \left(x_i^U - x_i^L\right)^2}{8}. \tag{14}$$

By replacing $\alpha$ with $\underline{\alpha}$, we get

$$d_{\alpha BB}^{\max}(\underline{\alpha}) = \sum_{i=1}^{n} \left( \frac{8\underline{\sigma_i}}{(x^U - x^L)^2} \right) \left( \frac{2\ln\left(\frac{3}{2}\right)}{\ln(2)} - 1 \right) \frac{\left(x_i^U - x_i^L\right)^2}{8} \tag{15}$$

$$= \sum_{i=1}^{n} \underline{\sigma_i} \left( \frac{2\ln\left(\frac{3}{2}\right)}{\ln(2)} - 1 \right) = d^{\max}(\underline{\sigma}). \tag{16}$$

□

**Theorem 12.** *Let $\overline{\alpha} = (\overline{\alpha_1}, \ldots, \overline{\alpha_n})$ be computed by using (3), then for $\overline{\sigma} = (\overline{\sigma_1}, \ldots, \overline{\sigma_n})$ where*

$$\overline{\sigma_i} = \frac{\overline{\alpha_i}}{8} \left(x_i^U - x_i^L\right)^2 \left( \frac{1}{\left( \frac{2\ln\left(\frac{3}{2}\right)}{\ln(2)} - 1 \right)} \right), \tag{17}$$

*$LB(x)$ and $LB_\alpha(x)$ have the same maximum separation distance between them and the function $f(x)$ for $\overline{\sigma}$ and $\overline{\alpha}$.*

*Proof.* The maximum separation distance between $LB(x)$ and $f(x)$ is given by

$$d^{\max}(\sigma) = \sum_{i=1}^{n} \sigma_i \left( \frac{2\ln\left(\frac{3}{2}\right)}{\ln(2)} - 1 \right). \tag{18}$$

By replacing $\sigma$ with $\overline{\sigma}$, we get

$$d^{\max}(\overline{\sigma}) = \sum_{i=1}^{n} \frac{\overline{\alpha_i}}{8} \left(x_i^U - x_i^L\right)^2 \left( \frac{1}{\left( \frac{2\ln\left(\frac{3}{2}\right)}{\ln(2)} - 1 \right)} \right) \left( \frac{2\ln\left(\frac{3}{2}\right)}{\ln(2)} - 1 \right) \tag{19}$$

$$= \sum_{i=1}^{n} \frac{\overline{\alpha_i} \left(x_i^U - x_i^L\right)^2}{8} = d_{\alpha BB}^{\max}(\overline{\alpha}). \tag{20}$$

□

### 3.3. Example

From an example in [2], we consider the following function:

$$f(x_1, x_2) = \cos(x_1)\cos(x_2) - \frac{x_1}{x_2^2 + 1},$$

where $x_1 \in [-1, 2]$ and $x_2 \in [-1, 1]$. We compute the following parameters:

| $i$ | $\underline{\alpha}$ | $\overline{\alpha}$ | $\underline{\sigma}$ | $\overline{\sigma}$ | $K_q$ |
|---|---|---|---|---|---|
| 1 | 1.5947 | 2.11551 | 10.5578 | 14.0059 | 26.9459 |
| 2 | 21.2511 | 28.1916 | 62.531 | 82.953 | 26.9459 |

Now we use the algorithm from [3]. For $\sigma = (12.7749, 75.6625)$, the new underestimator $LB(x)$ is convex. The minimum values for different underestimators are given in the following table:

| | $LB_q(x)$ | $LB_\alpha(x)$ | $LB(x)$ |
|---|---|---|---|
| Minimum value | $-43.89$ | $-17.1$ | $-15.79$ |

Table 1. Collection of multivariate test problems.

| | Source | Function | Domain ($n$) |
|---|---|---|---|
| 1 | [13] | $-\sin(x_1)\sin(x_1x_2)$ | $[0,4]^2$ |
| 2 | [13] | $-\sin(2x_1+x_2)/(\sin(x_2)+2)$ | $[-5,5]^2$ |
| 3 | [13] | $\sin(x_1+x_2)+(x_1-x_2)^2-1.5x_1+2.5x_2+1$ | $[-1.5,4]\times[-3,3]$ |
| 4 | [13] | $-\sin((x_1-1)(x_1-2)(x_2+1))$ | $[-1,1]\times[-2,0]$ |
| 5 | [13] | $(x1-1)^2+(x_2-1)^2+0.004/\left(1-x^{2/4}-x_2^2\right)+(x_1-2x_2+1)^2/0.4$ | $[1,2]^2$ |
| 6 | [13] | $\left(x_2-5x_1^2/(4\pi^2)+5x_1/\pi-6\right)^2+10(1-1/(8\pi))\cos(x_1)+10$ | $[-5,10]\times[0,15]$ |
| 7 | [13] | $100\left(x_2-x_1^2\right)+(x_1-1)^2$ | $[-3,3]\times[-1.5,4.5]$ |
| 8 | [13] | $0.1\left(12+x_1^2+\left(1+x_2^2\right)/x_1^2\right)+\left((x_1x_2)^2+100\right)/(x_1x_2)^4$ | $[1,3]^2$ |
| 9 | [13] | $0.5\left(x_1^2+x_2^2\right)-\cos(10\ln(2x_1))\cos(10\ln(3x_1))+1$ | $[0.01,1]^2$ |
| 10 | [13] | $\left(1+(x_1+x_2+1)^2\left(19-14x_1+3x_1^2-14x_2+6x_1x_2+3x_2^2\right)\right)$ $\left(30+(2x_1-3x_2)^2\left(18-32x_1+12x_1^2+48x_2-36x_1x_2+27x_2^2\right)\right)$ | $[-2,2]^2$ |
| 11 | [10] | $x_1^4+x_2-\left(x_1+x_2^2\right)^2$ | $[1,3]\times[-1,1]$ |
| 12 | [10] | $(1+x_1-e^{x_2})^2$ | $[0,1]\times[0,2]$ |
| 13 | [10] | $(2x_1+x_2-3)^2+(x_1x_2-1)^2$ | $[0,4]^2$ |
| 14 | [6] | $4x_1^2-2.1x_1^4+\frac{1}{3}x_1^6+x_1x_2-4x_2^2+4x_2^4$ | $[-3,3]\times[-1.5,1.5]$ |
| 15 | [6] | $(x_1-1)^2+(x_2-1)^2+(x_1+2x_2-3)^2+(x_1+2x_2-3)^4$ | $[0,2]^2$ |
| 16 | [6] | $x_1^2-0.1\cos(5\pi x_1)+x_2^2-0.1\cos(5\pi x_2)$ | $[-1,1]^2$ |
| 17 | [6] | $\sum_{i=1}^{2}\left\{4x_i^2-2.1x_i^4+x_i^6/6+x_ix_{i+1}-4x_{i+1}^2+4x_{i+1}^4\right\}$ | $[-2,2]^3$ |
| 18 | [6] | $x_1x_2-x_2x_3-x_3x_4+x_1x_2x_3-x_1+x_4$ | $[0,1]^4$ |
| 19 | [6] | $100(x_2-x_1^2)^2+(1-x1)^2+90(x_4-x_3^2+(1-x_3^2))$ $+10.1\left((1-x_2)^2+(1-x_4)^2\right)+19.8((1-x_2)+(1-x_4))$ | $[0,1]^4$ |
| 20 | [6] | $0.4x_1^{2/3}x_3^{-2/3}+0.4x_2^{2/3}x_4^{2/3}+10-x_1-x_2$ | $[0.1,10]^4$ |
| 21 | [6] | $\frac{1}{2}\sum_{i=1}^{4}\left(x_i^4-16x_i^2+5x_i\right)$ | $[-5,2]^4$ |
| 22 | [6] | $(x_1+10x_2)^2+5(x_3-x_4)^2+(x_2-2x_3)^4+10(x_1-x_4)^4$ | $[0,1]^4$ |
| 23 | [7] | $-x_1x_2+x_2x_3x_4$ | $[0,1]^4$ |

TABLE 2. Comparison results of the lower bound values of the proposed convex underestimator $LB$, $LB_q$, $LB_\gamma$ and $LB_\alpha$ for the first sixteenth test problems listed in Table 1.

| Function | $\min LB_q(x)$ | $\min LB_\alpha(x)$ | $\min LB_\gamma(x)$ | $\min LB(x)$ |
|---|---|---|---|---|
| 1 | −77.81 | −165.341 | −165.341 | −124.492 |
| 2 | −250.226 | −225.067 | −225.067 | −181.931 |
| 3 | −31.644 | −15.494 | −15.494 | −12.815 |
| 4 | −71 | −66.527 | −66.527 | −52.202 |
| 5 | −13.263 | −13.22 | −13.22 | −10.269 |
| 6 | −2066.993 | −863.883 | −863.883 | −741.066 |
| 7 | −106972 | −17802.49 | −17802.49 | −13657 |
| 8 | −6494.082 | −2907.738 | −2907.738 | −2191.350 |
| 9 | −432700 | −427500 | −427500 | −374700 |
| 10 | −2.333e+09 | −2.064e+09 | −2.064e+09 | −1.65e+09 |
| 11 | −82.966 | −14.020 | −14.020 | −10.585 |
| 12 | −119.493 | −12.0439 | −12.0439 | −10.122 |
| 13 | −349.105 | −230.996 | −230.996 | −172.224 |
| 14 | −4716.441 | −994.813 | −998.067 | −803.998 |
| 15 | −658.205 | −213 | −213 | −186.407 |
| 16 | −24.4366 | −22.837 | −22.837 | −18.495 |

TABLE 3. Comparison of number of iterations for the proposed underestimator $LB$, $LB_\alpha$ and the quadratic underestimator $LB_q$ on finding the optimal global minimum of the first sixteenth test problems listed in Table 1.

| | $\epsilon$ | $N^o it\ LB_q$ | $N^o it\ LB_\alpha$ | $N^o it\ LB$ | $f^*$ |
|---|---|---|---|---|---|
| 1 | $1 \times 10^{-7}$ | 182 | 96 | **85** | −1 |
| 2 | $1 \times 10^{-7}$ | 629 | 325 | **306** | −1 |
| 3 | $1 \times 10^{-7}$ | 35 | 13 | **12** | −1.913223 |
| 4 | $2 \times 10^{-3}$ | 305 | 165 | **149** | −1.002037 |
| 5 | $1 \times 10^{-7}$ | 92 | 33 | **30** | 0.169043 |
| 6 | $1 \times 10^{-7}$ | 399 | 53 | **52** | 0.379702 |
| 7 | $1 \times 10^{-7}$ | 1719 | 603 | **540** | 0 |
| 8 | $1 \times 10^{-7}$ | 88 | 41 | **38** | 1.728338 |
| 9 | – | – | – | – | – |
| 10 | $1 \times 10^{-7}$ | 1464 | 1134 | **991** | 3 |
| 11 | $1 \times 10^{-7}$ | 22 | 4 | **4** | −4 |
| 12 | $1 \times 10^{-7}$ | 6976 | 99 | **30** | 0 |
| 13 | $1 \times 10^{-7}$ | 117 | 117 | **102** | 0 |
| 14 | $1 \times 10^{-7}$ | 378 | 67 | **58** | −1.032 |
| 15 | $1 \times 10^{-7}$ | 78 | 44 | **35** | 0 |
| 16 | $1 \times 10^{-7}$ | 72 | 76 | **68** | −0.2 |

**Notes.** In bold the smallest numbers of iterations to find the optimal solutions when comparing the different methods.

## 4. Computational results

In the next experiment, we present a comparison results of the proposed convex underestimator with different convex underestimators for solving a collection of global optimization problems found in the literature and cited in Table 1. In [7], the authors reveal that the most efficient underestimator in term of number of iterations in branch and bound algorithms, is the quadratic piecewise underestimator which is developed in [11]. Therefore, in

TABLE 4. Comparison of number of iterations for the proposed underestimator $LB$, $LB_\gamma$, $LB_\alpha$ and the quadratic piecewise underestimator $LB_{p_{(Ni)}}$ on finding the optimal global minimum of the test problems listed in Table 1, with $1 \times 10^{-7} \leq \epsilon \leq 1 \times 10^{-5}$.

| | $N^o it\ LB_\gamma$ | $N^o it\ LB_\alpha$ | $N^o it\ LB - P_{(2)}$ | $N^o it\ LB$ |
|---|---|---|---|---|
| 1 | 182 | 96 | **69** | 85 |
| 2 | 325 | 325 | **215** | 306 |
| 3 | 13 | 13 | **12** | **12** |
| 4 | 165 | 165 | **141** | 149 |
| 5 | 33 | 33 | 32 | **30** |
| 6 | 53 | 53 | **46** | 52 |
| 7 | 603 | 603 | 583 | **540** |
| 8 | 41 | 41 | **27** | 38 |
| 9 | – | – | – | – |
| 10 | 1134 | 1134 | **713** | 991 |
| 11 | 17 | 4 | **3** | 4 |
| 12 | 6976 | 99 | 90 | **30** |
| 13 | 538 | 117 | 106 | **102** |
| 14 | 67 | 67 | **58** | **58** |
| 15 | 44 | 44 | **32** | 35 |
| 16 | 76 | 76 | **62** | 68 |
| 17 | 65 | 65 | **59** | 65 |
| 18 | 114 | 114 | **66** | 114 |
| 19 | 28 | 28 | **11** | 26 |
| 20 | 412 | 412 | **236** | 412 |
| 21 | 36 | 36 | **19** | 36 |
| 22 | 382 | 382 | **148** | 381 |
| 23 | 441 | 441 | 443 | **441** |

**Notes.** In bold the smallest numbers of iterations to find the optimal solutions when comparing the different methods.

Table 4 we compare the number of iterations of the $\alpha$BB algorithm [5] when using the proposed underestimator $LB(x)$, $\alpha$BB underestimators $LB_\alpha(x)$ and $LB_\gamma(x)$, and the quadratic piecewise underestimator $LB - P_{(Ni)}(x)$.

The $\alpha$BB algorithm is implemented in C++ programs and executed on a Dell computer with an Intel(R) Core(TM) i5-4210U CPU with a speed of 3.40 GHz and 8 GB RAM.

The following criteria is taken in consideration:

- $N^o it$ is the number of iterations of the $\alpha$BB algorithm for each underestimator.

Table 2 shows that the proposed underestimator gives always better lower bound values than the quadratic and the classical $\alpha$BB underestimators, which proves the theoretical improvements of the proposed underestimator.

Table 3 indicates that the number of iterations of the $\alpha$BB algorithm when using the proposed underestimator is always better than the number of iterations obtained when using the quadratic or the classical $\alpha$BB underestimators for finding the optimal global minimum.

Table 4 shows that in many cases the proposed underestimator gives a better number of iterations compared to other underestimators even for higher dimensional problems.

## 5. Conclusion

In this work, we proposed a new convex underestimator for general nonconvex functions on a box. Theoretical and numerical results show that the new underestimator is tighter than the classical $\alpha$BB and the quadratic underestimators. Moreover, we have used this new convex underestimator and other underestimators in a Branch and bound algorithm, then we compared the performance results for solving global optimization problems found in the literature.

## Data availability statement

The code used in this paper is available online in the GitHub repository: https://github.com/zerroukidj/alphaBBalgorithm.git [15].

The libraries used in the implementation are available online:

– Boost C++ Libraries: https://www.boost.org/
– Eigen C++ Library: https://eigen.tuxfamily.org/index.php?title=Main_Page
– Nlopt C++ Library: https://nlopt.readthedocs.io/en/latest/

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