# A GLOBAL OPTIMIZATION METHOD, $\alpha$BB, FOR PROCESS DESIGN

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## Abstract

A global optimization algorithm, $\alpha$BB, for twice–differentiable NLPs is presented. It operates within a branch–and–bound framework and requires the construction of a convex lower bounding problem. A technique to generate such a valid convex underestimator for arbitrary twice–differentiable functions is described. The $\alpha$BB has been applied to a variety of problems and a summary of the results obtained is provided.

## 1 Introduction

In their search to arrive at better designs for new or existing processes, chemical engineers often need to solve nonconvex optimization problems. These problems arise in many areas, such as computational chemistry, phase equilibrium, process unit sequencing. Despite the importance of identifying the global minimum solution, or valid bounds on that solution, this can rarely be achieved rigorously. Global optimization has therefore been the focus of much interest in recent years (Floudas and Grossmann, 1995), (Floudas, 1995), (Floudas and Pardalos, 1996).

The construction of a convex underestimating problem, which allows the generation of two converging sequences of upper and lower bounds, emerges as central theme in many of the methods developed to date. In particular, the GOP algorithm (Visweswaran and Floudas, 1995a) and the branch–and–bound algorithm of Al-Khayyal and Falk (1983) rely on mathematical properties specific to the problem solved in order to obtain the lower bounding problem. Maranas and Floudas (1994a,b) and Androulakis *et al.* (1995) suggested an approach which necessitates the identification of the minimum eigenvalues of the functions to be convexified over the domain of interest. The $\alpha$BB algorithm, based on this technique, converges with mathematical rigor to the desired solution within some pre–set tolerance, and has been shown to be applicable to the broad class of twice–differentiable nonconvex programs (Liu and Floudas, 1993a). However, the exact calculation of the minimum eigenvalue of a general function over a given region of the variable space poses tremendous difficulties. The generation of a *valid lower bound* on that eigenvalue preserves the theoretical guarantees of global optimality while improving the tractability of the problem.

After an introduction to the basic concepts of the $\alpha$BB algorithm, a technique for the calculation of the eigenvalue lower bound is described. It exploits the properties of interval polynomials to achieve its goal. Finally, a summary of results for a number of standard optimization problems and some design problems is provided.

## 2 The $\alpha$BB algorithm

### 2.1 Basic Concepts

The $\alpha$BB global optimization algorithm can rigorously address general twice–differentiable NLPs, as shown in equation (2.1).

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$$\begin{array}{lrcl} \min\limits_{\mathbf{x}} & f(\mathbf{x}) & & \\ s.t. & \mathbf{g}(\mathbf{x}) & \leq & 0 \\ & \mathbf{h}(\mathbf{x}) & = & 0 \\ & \mathbf{x} & \in & X \subseteq \Re^n \end{array} \tag{2.1}$$

where $f$, $\mathbf{g}$ and $\mathbf{h}$ belong to $\mathcal{C}^2$, the set of twice-differentiable functions, and $\mathbf{x}$ is a vector of size $n$.

The method is based on a branch–and–bound strategy, in which the design of a lower bounding scheme plays a crucial part. Convergence to the global optimum is achieved only if the lower bounds generated are *valid* and they form a *nondecreasing* sequence. Yet, in order to ensure satisfactory computational times, the underestimating problem should be constructed to be as tight as possible. To meet these requirements, the functions in the problems are decomposed into a sum of terms. Depending on its mathematical structure, each term is then assigned to one of several pre–defined categories. The advantage of this method is that each class of terms can be underestimated using a known and effective technique. The special classes of terms considered here are linear, convex, bilinear, and univariate concave terms. For the first two categories, no underestimator is required, while for the third one, the convex envelope (Al-Khayyal and Falk, 1983) is used. For the last class, a linearization is used. Any term that does not fall within one of these classes is labelled as a general nonconvex term.

A twice–differentiable nonconvex function $f(\mathbf{x})$ can therefore be expressed as

$$f(\mathbf{x}) = LT(\mathbf{x}) + CT(\mathbf{x}) + \sum_{i=1}^{bt} b_i x^{i,1} x^{i,2} + \sum_{i=1}^{ut} UT_i(x^i) + \sum_{i=1}^{nt} NT_i(\mathbf{x})$$

where $LT(\mathbf{x})$ is a linear term, $CT(\mathbf{x})$ is a convex term, $bt$ is the number of bilinear terms, $x^{i,1}$ and $x^{i,2}$ denote the two variables that participate in the $i$th bilinear term, $b_i$ is the coefficient of the $i$th bilinear term, $ut$ is the number of univariate concave terms, $UT_i(x^i)$ is the $i$th univariate concave term, $x^i$ denotes the variable that participates in $UT_i$, $nt$ is the number of general nonconvex terms, $NT_i(\mathbf{x})$ is the $i$th general nonconvex term.

Its convex underestimator then takes the following form :

$$\begin{aligned} \mathcal{L}(\mathbf{x},\mathbf{w}) = \; & LT(\mathbf{x}) + CT(\mathbf{x}) + \sum_{i=1}^{bt} b_i w_i \\ & + \sum_{i=1}^{ut} \left( UT_i(x^{i,L}) + \frac{UT_i(x^{i,U}) - UT_i(x^{i,L})}{x^{i,U} - x^{i,L}} (x - x^{i,L}) \right) \\ & + \sum_{i=1}^{nt} \left( NT_i(\mathbf{x}) + \sum_{j=1}^{n} \alpha_{ij} (x_j - x_j^L)(x_j - x_j^U) \right) \end{aligned} \tag{2.2}$$

where

$$\begin{aligned} w_i \geq \max\{ \; & x^{i,1,L} x^{i,1} + x^{i,2,L} x^{i,2} - x^{i,1,L} x^{i,2,L}; \\ & x^{i,1,U} x^{i,1} + x^{i,2,U} x^{i,2} - x^{i,1,U} x^{i,2,U} \}, \text{ for } i = 1, \cdots, bt. \end{aligned}$$

and

$$\begin{aligned} \alpha_{ij} & \geq \max\{0, -\tfrac{1}{2} \min_{k, \mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U} \lambda_{j,k}(\mathbf{x})\}, \text{ if } NT_j(\mathbf{x}) \text{ is a function of } x_i \text{ or,} \\ \alpha_{ij} & = 0 \text{ otherwise (see Maranas and Floudas, 1994a, b),} \end{aligned} \tag{2.3}$$

where the $\lambda_{j,k}(\mathbf{x})$'s are the eigenvalues of the term $NT_j(\mathbf{x})$ and the superscripts $L$ and $U$ denote the lower and upper bounds on the variables, respectively.

In the light of equations (2.2) and (2.3), the only remaining difficulty in the construction of a valid convex underestimator is the determination of the parameter $\alpha$ or, equivalently, of a bound on the minimum eigenvalue of a general nonconvex term. This problem is addressed in the following section.

## 2.2 Rigorous calculation of $\alpha$

The proposed technique for the calculation of a rigorous lower bound on the minimum eigenvalue $\lambda_{min}$ of an arbitrary twice–differentiable function $f(\mathbf{x})$ is based on the derivation of its interval characteristic polynomial and the use of some properties of interval polynomials. Before the methodology is outlined and tested, several definitions and properties are introduced.

By definition, the characteristic polynomial of a function $f(\mathbf{x})$ is obtained by deriving the Hessian matrix $H(\mathbf{x})$ of $f(\mathbf{x})$ and then taking the determinant of $H(\mathbf{x}) - \lambda I$ where $I$ is the identity matrix. The general form of the characteristic polynomial is therefore expressed as

$$\mathcal{P}_f(\mathbf{x}, \lambda) = a_0(\mathbf{x}) + a_1(\mathbf{x})\lambda + \cdots + a_{n-1}(\mathbf{x})\lambda^{n-1} + \lambda^n \tag{2.4}$$

**Definition 1** $\mathcal{P}_f(\mathbf{x}, \lambda)$ as defined in (2.4) describes a *family of polynomials* : for each combination of the values of the coefficients, a polynomial $\mathcal{P}_f(\lambda)$ is formed.

**Definition 2** If the real parts of all the roots of the polynomials in a family lie in the right–half plane, then this polynomial family is said to be *anti–stable.*

**Property 1** *The function $f(\mathbf{x})$ is convex over the domain $X$ if and only if the polynomial family $\mathcal{P}_f(\mathbf{x}, \lambda)$ is anti–stable over $X$.*

In order to simplify the problem of determining the stability characteristics of $\mathcal{P}_f(\mathbf{x}, \lambda)$, the following definition is introduced.

**Definition 3** An *interval polynomial family* is a family represented by a polynomial whose coefficients are not scalars but intervals.

Using the fundamental concepts of interval analysis as presented in Ratschek and Rokne (1988) and Neumaier (1990), the characteristic polynomial $\mathcal{P}_f(\mathbf{x}, \lambda)$ of a function $f(\mathbf{x})$ over the region $X = [\mathbf{x}^L, \mathbf{x}^U]$ can be transformed into an interval polynomial family $\mathcal{P}_{f,X}(\lambda)$.

$$\mathcal{P}_{f,X}(\lambda) = [a_0^L, a_0^U]\lambda + [a_1^L, a_1^U]\lambda + \cdots + [a_{n-1}^L, a_{n-1}^U]\lambda^{n-1} + \lambda^n \tag{2.5}$$

where $a_i^L \le a_i(\mathbf{x}) \le a_i^U, \ \forall i, \ \mathbf{x} \in [\mathbf{x}^L, \mathbf{x}^U]$.
$\mathcal{P}_{f,X}(\lambda)$ specifies a family of polynomials that contains the set of polynomials $\mathcal{P}_f(\mathbf{x}, \lambda)$. Note that if the coefficients of $\mathcal{P}_f(\mathbf{x}, \lambda)$ are independent, then $\mathcal{P}_f(\mathbf{x}, \lambda) = \mathcal{P}_{f,X}(\mathbf{x})$.

**Property 2** *$\mathcal{P}_{f,X}(\lambda)$ anti–stable $\Rightarrow$ $f(\mathbf{x})$ convex over $X$.*

Although Property 2 allows to test the convexity of the function $f$ over a specific domain, it does not provide an estimate of the smallest eigenvalue. The concept of *margin of anti–stability* is borrowed from control theory in order to obtain the desired lower bound.

**Property 3** *Let $\lambda_{min}$ be the smallest root of $\mathcal{P}_{f,X}(\lambda)$. Then $\lambda^* = \lambda_{min}$ is the smallest value for which $\mathcal{P}_{f,X}(\lambda - \lambda^*)$ is anti–stable. Thus the margin of anti–stability of $\mathcal{P}_{f,X}(\lambda)$ is $\lambda_{min}$.*

Finding $\lambda_{min}$ can then be expressed as the following optimization problem :

$$\lambda_{min} = \left\{ \begin{array}{ll} \min\limits_{\lambda, \lambda^*} & \lambda^* \\ s.t. & \mathcal{P}_{f,X}(\lambda - \lambda^*) \text{ anti} - \text{stable} \end{array} \right\} \tag{2.6}$$

Problem (2.6) can be reduced to a simpler form if the Kharitonov theorem is used (Kharitonov, 1979). The stability of an interval polynomial family can be determined by testing the stability of only four of the polynomials in the family. Based on the relationship between stability and anti–stability, the Kharitonov polynomials can also be used to test anti–stability of an interval polynomial family.

**Property 4** *If the polynomials*

$$\begin{array}{l} K_1(f, X, \lambda) = a_0^L + a_1^L\lambda + a_2^U\lambda^2 + a_3^U\lambda^3 + a_4^L\lambda^4 + a_5^L\lambda^5 + a_6^U\lambda^6 + \cdots \\ K_2(f, X, \lambda) = a_0^U + a_1^U\lambda + a_2^L\lambda^2 + a_3^L\lambda^3 + a_4^U\lambda^4 + a_5^U\lambda^5 + a_6^L\lambda^6 + \cdots \\ K_3(f, X, \lambda) = a_0^U + a_1^L\lambda + a_2^L\lambda^2 + a_3^U\lambda^3 + a_4^U\lambda^4 + a_5^L\lambda^5 + a_6^L\lambda^6 + \cdots \\ K_4(f, X, \lambda) = a_0^L + a_1^U\lambda + a_2^U\lambda^2 + a_3^L\lambda^3 + a_4^L\lambda^4 + a_5^U\lambda^5 + a_6^U\lambda^6 + \cdots \end{array} \tag{2.7}$$

*are anti–stable then the polynomial family $\mathcal{P}_{f,X}(\lambda)$ is anti–stable.*

Combining properties 3 and 4, Problem (2.6) can now be solved by the following procedure :

- Construct the four Kharitonov polynomials $K_1(f,X,\lambda)$, $K_2(f,X,\lambda)$, $K_3(f,X,\lambda)$ and $K_4(f,X,\lambda)$.
- Calculate all the roots of these polynomials. The smallest root is $\lambda_{min}$.

The above procedure yields a valid lower bound on the minimum eigenvalue of $f(\mathbf{x})$ for $\mathbf{x} \in X$. Note that the only dependence on the number of independent variables arises during the stability check : the number of roots of each Kharitonov polynomial is equal to the number of variables. The roots can be obtained efficiently since the Kharitonov polynomials involve a single variable.

Finally, the accuracy of the lower bound obtained can be increased if the interdependence of the coefficients of the characteristic polynomials is taken into account, as proposed by Bartlett *et al.* (1987) for the case of linearly dependent coefficients. However, such a technique greatly increases computational expense and a compromise must be achieved between efficiency and accuracy.

**Small Example** Consider $f(x_1,x_2) = x_1^3 - x_1x_2^2$ with $(x_1,x_2) \in X = [0,1]^2$. Its characteristic polynomial is $-12x_1^2 - 4x_2^2 - 4x_1\lambda + \lambda^2 = 0$. Its interval characteristic polynomial over X is $[-16,0] + [-4,0]\lambda + \lambda^2 = 0$ The four Kharitonov polynomials are then :

$$\begin{array}{ll} K_1(f,X,\lambda) = -16 - 4\lambda + \lambda^2 & K_2(f,X,\lambda) = \lambda^2 \\ K_3(f,X,\lambda) = -4\lambda + \lambda^2 & K_4(f,X,\lambda) = -16 + \lambda^2 \end{array}$$

The set of the roots of these polynomials is $\{-4, 2-2\sqrt{5}, 0, 4, 2+2\sqrt{5}\}$. Thus the computed lower bound on the minimum eigenvalue of $f(x_1,x_2)$ over $X$ is -4. The exact value of $\lambda_{min}$ was found to be -2.5 using GAMS.

**Illustrative Example** The potential energy function for the pseudoethane molecule is especially interesting since it is highly nonlinear and is expressed in terms of only one variable, the dihedral angle (equation (2.2)). It is used to present a visual interpretation of the proposed method. Underestimators of the potential function were built for different domains of the variable space, using the calculated lower bound on the minimum eigenvalue. For each level of partition, the resulting convex piecewise underestimator was drawn, as shown in Figure (1). It can be seen that, although the initial lower bounds are very loose, they improve rapidly to provide a good approximation of the original function.

$$\begin{aligned} f(t) = \; & \frac{588600}{\left(3\,r_0^2 - 4\cos\theta r_0^2 - 2\left(\sin^2\theta\cos(t-\frac{2\pi}{3}) - \cos^2\theta\right)r_0^2\right)^6} - \frac{1079.1}{\left(3\,r_0^2 - 4\cos\theta r_0^2 - 2\left(\sin^2\theta\cos(t-\frac{2\pi}{3}) - \cos^2\theta\right)r_0^2\right)^3} \\ & + \frac{600800}{\left(3\,r_0^2 - 4\cos\theta r_0^2 - 2\left(\sin^2\theta\cos(t) - \cos^2\theta\right)r_0^2\right)^6} - \frac{1071.5}{\left(3\,r_0^2 - 4\cos\theta r_0^2 - 2\left(\sin^2\theta\cos(t) - \cos^2\theta\right)r_0^2\right)^3} \\ & + \frac{481300}{\left(3\,r_0^2 - 4\cos\theta r_0^2 - 2\left(\sin^2\theta\cos(t+\frac{2\pi}{3}) - \cos^2\theta\right)r_0^2\right)^6} - \frac{1064.6}{\left(3\,r_0^2 - 4\cos\theta r_0^2 - 2\left(\sin^2\theta\cos(t+\frac{2\pi}{3}) - \cos^2\theta\right)r_0^2\right)^3} \end{aligned}$$

where $r_0$ is the covalent bond length ($1.54\mathring{A}$), $\theta$ is the covalent bond angle ($109.5^o$), and $t$ is the dihedral angle ($0 \leq t \leq 2\pi$).

# 3 Summary of Computational Results

The $\alpha$BB algorithm has been implemented in a flexible and user–friendly format and it has been used to successfully solve a large number of examples. Table (1) summarizes the results obtained for a sample of literature and design problems. The HP (Haverly pooling) problems are a set of bilinearly constrained problems, while the LCP problems are linearly constrained concave programs. NLP is a small yet highly nonconvex test problem. The remaining formulations represent chemical engineering design problems. RN1 corresponds to the optimization of a small reactor problem, while RN2 is a more complex reactor network synthesis for the *Van der Vusse* reaction. HEN corresponds to the design of a network of three heat exchanger. Finally, SEP is a superstructure optimization problem for a separation system with two units.

# 4 Conclusion

A sufficient condition for the generation of a lower bound on the minimum eigenvalue of a twice–differentiable function was presented. Using the Kharitonov theorem and the interval characteristic polynomial of the function, an iterative scheme has been devised to calculate the desired value. The $\alpha$BB global optimization algorithm has been implemented and used effectively to solve problems from the very broad class of twice–differentiable NLPs.

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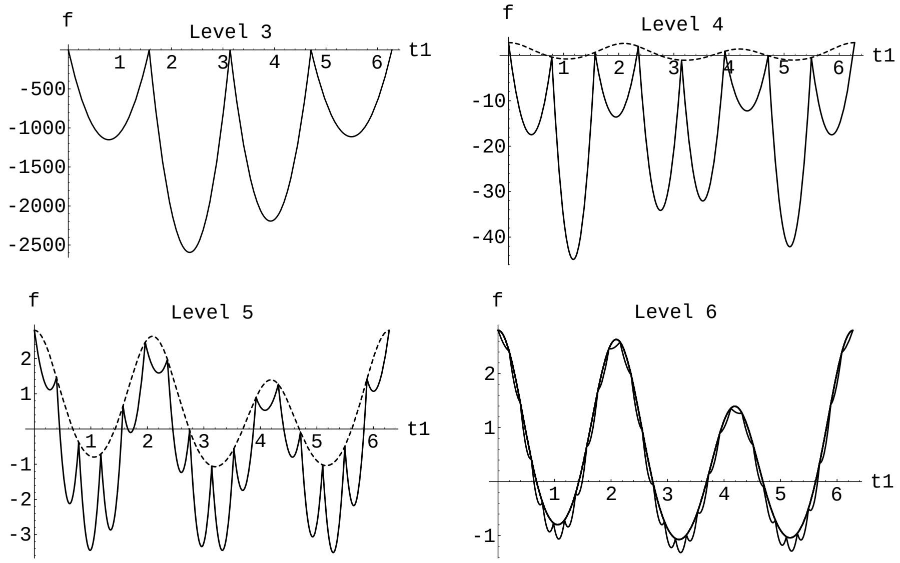


Figure 1: Function and underestimator at different levels of the branch–and–bound tree using calculated $\alpha$ values

| Problem Name | Reference | Number of variables | Number of constraints | $N_i$ | $N_n$ | CPU time (s) |
|---|---|---|---|---|---|---|
| HP1 | Floudas and Pardalos (1990) | 9 | 6 | 13 | 27 | 1.31 |
| HP2 | Floudas and Pardalos (1990) | 9 | 6 | 17 | 35 | 1.56 |
| HP3 | Floudas and Pardalos (1990) | 9 | 6 | 9 | 19 | 1.08 |
| LCP1 | Floudas and Pardalos (1990) | 20 | 10 | 30 | 61 | 7.03 |
| LCP2 | Floudas and Pardalos (1990) | 20 | 10 | 25 | 51 | 6.07 |
| LCP3 | Floudas and Pardalos (1990) | 20 | 10 | 30 | 61 | 6.66 |
| LCP4 | Floudas and Pardalos (1990) | 20 | 10 | 26 | 53 | 6.38 |
| LCP5 | Floudas and Pardalos (1990) | 20 | 10 | 82 | 165 | 16.5 |
| NLP | Murtagh and Saunders (1988) | 5 | 3 | 232 | 465 | 99.6 |
| RN1 | Ryoo and Sahinidis (1995) | 6 | 5 | 48 | 97 | 13.8 |
| RN2 | Floudas and Pardalos (1990) | 29 | 45 | 154 | 308 | 1988 |
| HEN | Floudas and Pardalos (1990) | 8 | 6 | 133 | 267 | 23.4 |
| SEP | Floudas and Aggarwal (1990) | 38 | 49 | 101 | 203 | 494 |

Table 1: Summary of computational results ($N_i$, number of iterations, $N_n$, number of expanded nodes)