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Convex Underestimation of Twice Continuously Differentiable Functions by Piecewise Quadratic Perturbation: Spline αBB Underestimators

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Abstract. This paper describes the construction of convex underestimators for twice continuously differentiable functions over box domains through piecewise quadratic perturbation functions. A refinement of the classical αBB convex underestimator, the underestimators derived through this approach may be significantly tighter than the classical αBB underestimator. The convex underestimator is the difference of the nonconvex function f and a smooth, piecewise quadratic, perturbation function, q. The convexity of the underestimator is guaranteed through an analysis of the eigenvalues of the Hessian of f over all subdomains of a partition of the original box domain. Smoothness properties of the piecewise quadratic perturbation function are derived in a manner analogous to that of spline construction.

Key words: αBB, Convex underestimator, Global optimization, Splines

1. Introduction

In this paper the convex underestimation of C^2 continuous functions is investigated. This work extends and refines the convex underestimation approach used in the αBB global optimization algorithm developed by Maranas and Floudas (1994), Adjiman et al. (1996, 1998a, b), and Floudas (2000). The αBB algorithm is based on the idea of constructing a smooth convex underestimator of a nonconvex C^2 continuous function, $f : \mathbb{R}^n \to \mathbb{R}$, using a convex quadratic perturbation function, $q : \mathbb{R}^n \to \mathbb{R}$. The convex underestimator $\phi : \mathbb{R}^n \in x \to \mathbb{R}$ is defined as follows:

$$\phi(x) := f(x) - q(x).$$

The αBB convexification approach can be viewed as an approximate solution to a more general convexification problem, that of finding a convexifying perturbation function $q(x)$ which minimizes a measure, μ, of the separation between a nonconvex C^2 continuous function $f(x)$ and the convex underestimator $f(x) - q(x)$. This can be stated in the form,

$$\min_q \mu(q(x))$$
subject to
$$\nabla^2(f(x) - q(x)) \succeq 0 \quad \text{for all } x \in \mathbf{x},$$
$$q(x) \geqslant 0 \quad \text{for all } x \in \mathbf{x},$$

where $\mathbf{x} \subset \mathbb{R}^n$ denotes the hyperrectangle defined by upper and lower bounds on the elements of x, that is $\mathbf{x} := [\underline{x}_1, \bar{x}_1] \times \cdots \times [\underline{x}_n, \bar{x}_n]$. The relation $\nabla^2(f(x) - q(x)) \succeq 0$ means that $\nabla^2(f(x) - q(x))$ is *positive semidefinite*. The objective function may be $-q(x)$, the separation distance, or some other measure such as the overestimation volume $\int_{\mathbf{x}} -q(x)\, \mathrm{d}x$. This optimization problem may have a solution functional $q^*(x)$ which is nondifferentiable and nonconvex.
In the classical αBB approach, a series of simplifications are made to yield an efficient convexification procedure. The first of these simplications is the imposition of a quadratic structure on the perturbation function,

$$q(x) := \sum_{i=1}^{n} \alpha_i (\bar{x}_i - x_i)(x_i - \underline{x}_i).$$

To ensure that $q(x)$ is nonnegative, α is assumed to be nonnegative. Observe that $q(x)$, a quadratic function with a diagonal Hessian matrix

$$\nabla^2 q(x) := 2 \ \mathrm{diag}(\alpha)$$

has an eigenvalue–eigenvector structure that is uniform over the entire domain $\mathbf{x}$ with eigenvectors that are aligned with the coordinate axes. In the work of Adjiman et al. (1998b) a second simplification is introduced in which the *interval extension* $\mathbf{H}^{\mathbf{x}}$ is used instead of $\nabla^2 f(x)$ itself. The interval extension of the matrix $\nabla^2 f(x) \in \mathbb{R}^{n \times n}$ is a matrix of intervals of $\mathbb{R}$. Each element $\mathbf{H}^{\mathbf{x}}_{ij}$ of the matrix $\mathbf{H}^{\mathbf{x}}$ is defined in such a way that

$$\left. \frac{\partial^2 f}{\partial x_i \, \partial x_j} \right|_x \in \mathbf{H}^{\mathbf{x}}_{ij} \quad \text{for all } x \in \mathbf{x}.$$

Computing the tightest possible interval extension is in itself a global optimization problem. In practice an interval extension can be calculated using interval arithmetic (Moore, 1966; Ratschek and Rokne, 1984; Neumaier, 1990). The overestimation made in the interval calculations may result in a significant loss of accuracy. Adjiman et al. (1998b) applied the work of Gerschgorin (1931), Deif (1991), Rohn (1996), Mori and Kokame (1994), Stephens (1997), Kharitonov (1979), Hertz (1992) and Neumaier (1992) to compute α vectors that guarantee the convexity of the underestimator. The tightness of the underestimator is dependent on the particular α calculation method.

In NLP and MINLP applications the number of variables that participate in a given nonconvex function is usually considerably less than the total number of variables participating in the complete set of nonconvex functions. Any relaxation based branch and bound algorithm such as the αBB is such that the refinement of the convex underestimator of any nonconvex constraint is contingent on the reduction of the domain of a variable participating in that constraint. Consider, for example, the NLP

$$\min_{x \in \mathbf{x}} f(x_5)$$
subject to
$$g_1(x_1, x_2) \leqslant 0,$$
$$g_2(x_2, x_3) \leqslant 0,$$
$$g_3(x_3, x_4) \leqslant 0,$$
$$g_4(x_4, x_5) \leqslant 0$$

in which f and $g_i, i = 1, \ldots, 4$ are C^2 continuous nonconvex functions. Within the αBB framework each of these functions would be replaced by a convex underestimator. To improve the underestimation of f, branching on x_5 would need to occur, but this would not improve the underestimation of g_1, g_2, or g_3. Only after branching on x_2, x_3 and x_5 would the convex underestimator of the objective and each constraint be refined. In the process the branch and bound tree would be expanded and a number of convex optimization problems would have to be solved. If the convex underestimators could be refined efficiently and without branching a more efficient global optimization would result. In this paper the form of the αBB perturbation function and the way in which it is calculated are reexamined, a novel spline based method for convex underestimation is proposed and an efficient means of computing these tighter underestimators is elucidated.

The remainder of this paper is structured as follows. In Section 2 the form of the new convex underestimator is introduced. A geometrical interpretation of this underestimator is presented in Section 3. Properties of this function are proven in Section 4. Section 5 discusses a modification of this underestimator which relaxes the requirement that the α values be positive. The implementation of this underestimation approach is discussed in Section 6 and computational results are provided in Section 7.

2. An α Spline Underestimator

The size of the domain $\mathbf{x}$ effects the result of every step in the α calculation and strongly influences the tightness of the resulting convex underestimator. In particular, reducing $\mathbf{x}$ reduces the mismatch between the assumed quadratic functional form and the ideal form; it reduces the overestimation in the interval extension of the Hessian matrix; and the maximum separation distance has been shown to be a quadratic function of interval length (Maranas and Floudas, 1994). It is therefore useful to construct a convex underestimator using a number of different α vectors, each applying to a *subregion* of the full domain $\mathbf{x}$.

Let $f(x) : \mathbb{R}^n \to \mathbb{R}$ be a C^2 continuous function. For each variable $x_i \in \mathbb{R}$ let the interval $[\underline{x}_i, \bar{x}_i]$ be partitioned into N_i subintervals. The endpoints of these subintervals are denoted $x_i^0, x_i^1, \ldots, x_i^{N_i}$ where $\underline{x}_i = x_i^0 < x_i^1 < \cdots < x_i^k < \cdots < x_i^{N_i} = \bar{x}_i$. In this notation the kth interval is $[x_i^{k-1}, x_i^k]$. A smooth convex underestimator of $f(x)$ over $\mathbf{x}$ is defined by

$$\phi(x) := f(x) - q(x),$$

where

$$q(x) := \sum_{i=1}^{n} q_i^k(x_i) \quad \text{for } x_i \in [x_i^{k-1}, x_i^k], \tag{1}$$

$$q_i^k(x_i) := \alpha_i^k(x_i - x_i^{k-1})(x_i^k - x_i) + \beta_i^k x_i + \gamma_i^k. \tag{2}$$

In each interval $[x_i^{k-1}, x_i^k], \alpha_i^k \geqslant 0$ is chosen such that $\nabla^2\phi(x)$, the Hessian matrix of $\phi(x)$, is positive semidefinite for all members of the set $\{x \in \mathbf{x} : x_i \in [x_i^{k-1}, x_i^k]\}$. $q_i^k(x_i)$ is the quadratic function associated with variable i in interval k. The function $q(x)$ is a piecewise quadratic function constructed from the functions $q_i^k(x_i)$.

The continuity and smoothness properties of $q(x)$ are produced in a spline-like manner. For $q(x)$ to be smooth the q_i^k functions and their gradients must match at the endpoints x_i^k. In addition, we require that $q(x) = 0$ at the vertices of the hyperrectangle $\mathbf{x}$. To satisfy these requirements, the following conditions are imposed for all $i = 1, \ldots, n$:

$$q_i^1(x_i^0) = 0, \tag{3}$$

$$q_i^k(x_i^k) = q_i^{k+1}(x_i^k) \quad \text{for all } k = 1, \ldots, N_i - 1, \tag{4}$$

$$q_i^{N_i}(x_i^{N_i}) = 0, \tag{5}$$

$$\left.\frac{\mathrm{d}q_i^k}{\mathrm{d}x_i}\right|_{x_i^k} = \left.\frac{\mathrm{d}q_i^{k+1}}{\mathrm{d}x_i}\right|_{x_i^k} \quad \text{for all } k = 1, \ldots, N_i - 1. \tag{6}$$

Expanding these equations, for each $i = 1, \ldots, n$, one obtains the following system of equations:

$$\beta_i^1 x_i^0 + \gamma_i^1 = 0,$$
$$\beta_i^k x_i^k + \gamma_i^k = \beta_i^{k+1} x_i^k + \gamma_i^{k+1} \quad \forall k = 1, \ldots, N_i - 1,$$
$$\beta_i^{N_i} x_i^{N_i} + \gamma_i^{N_i} = 0,$$
$$-\alpha_i^k (x_i^k - x_i^{k-1}) + \beta_i^k = \alpha_i^{k+1}(x_i^{k+1} - x_i^k) + \beta_i^{k+1} \quad \forall k = 1, \ldots, N_i - 1,$$

which can be represented as,

$$\begin{bmatrix} -x_i^0 & & & & & & -1 & & & & \\ x_i^1 & -x_i^1 & & & & & 1 & -1 & & & \\ & \ddots & \ddots & & & & & \ddots & \ddots & & \\ & & x_i^k & -x_i^k & & & & & 1 & -1 & \\ & & & \ddots & \ddots & & & & & \ddots & \ddots \\ & & & & x_i^{N_i} & & & & & & 1 \\ -1 & 1 & & & & & & & & & \\ & -1 & 1 & & & & & & & & \\ & & \ddots & \ddots & & & & & & & \\ & & & -1 & 1 & & & & & & \end{bmatrix} \begin{bmatrix} \beta_i^1 \\ \beta_i^2 \\ \vdots \\ \beta_i^k \\ \vdots \\ \beta_i^{N_i} \\ \gamma_i^1 \\ \gamma_i^2 \\ \vdots \\ \gamma_i^{N_i} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \\ s_1 \\ s_2 \\ \vdots \\ s_i^{N_i - 1} \end{bmatrix},$$

where $s_i^k = -\alpha_i^k (x_i^k - x_i^{k-1}) - \alpha_i^{k+1}(x_i^{k+1} - x_i^k)$. As the solution one obtains

$$\beta_i^1 = \left(\sum_{k=1}^{N_i - 1} s_i^k (x_i^k - x_i^{N_i}) \right) \Big/ \left(x_i^{N_i} - x_i^0 \right), \tag{7}$$

$$\beta_i^k = \beta_i^1 + \sum_{j=1}^{k-1} s_i^j \quad \text{for all } k = 2, \ldots, N_i, \tag{8}$$

$$\gamma_i^k = -\beta_i^1 x_i^0 + \sum_{j=1}^{k-1} s_i^j x_i^j \quad \text{for all } k = 1, \ldots, N_i. \tag{9}$$

3. Geometric Interpretation

The construction of the convex underestimator for a nonconvex function

$$f(x) = -2x + 10x^2 - 3x^3 - 5x^4$$

over the domain $x \in [0, 1]$ is illustrated in Figures 1 and 2. Figure 2 shows the nonconvex function $f(x)$ along with underestimators of $f(x)$. A convex underestimator defined using the classical αBB approach requires the α value to be large enough to cancel the negative curvature at *all* points in the domain. Noting that the second derivative, $f''(x) = 20 - 18x - 60x^2$, is a

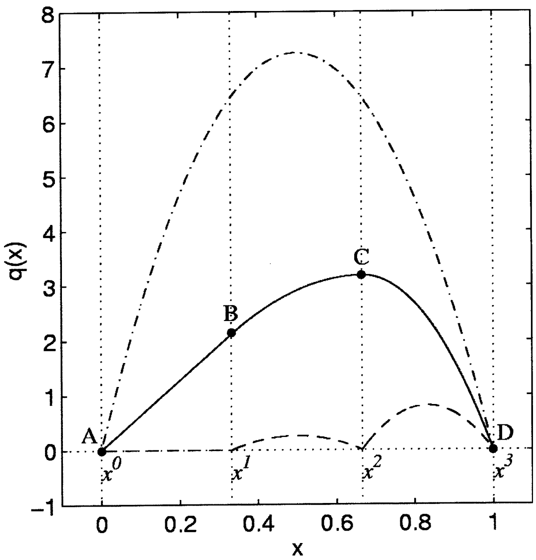

Figure 1. Geometric interpretation of conditions (A) $q^1(x^0) = 0$, (B) $q^1(x^1) = q^2(x^1)$ and $\frac{dq^1}{dx}\big|_{x^1} = \frac{dq^2}{dx}\big|_{x^1}$, (C) $q^2(x^2) = q^3(x^2)$ and $\frac{dq^2}{dx}\big|_{x^2} = \frac{dq^3}{dx}\big|_{x^2}$ and (D) $q^3(x^3) = 0$. αBB underestimator (-·-), αBB underestimators over partial domains (– –), piecewise underestimator (–).

monotonically *decreasing* function of x, the most negative curvature occurs at $x = 1$, hence the α parameter is defined by $f''(1)$ using the formula,

$$\alpha = -\frac{1}{2}f''(1) = 29.$$

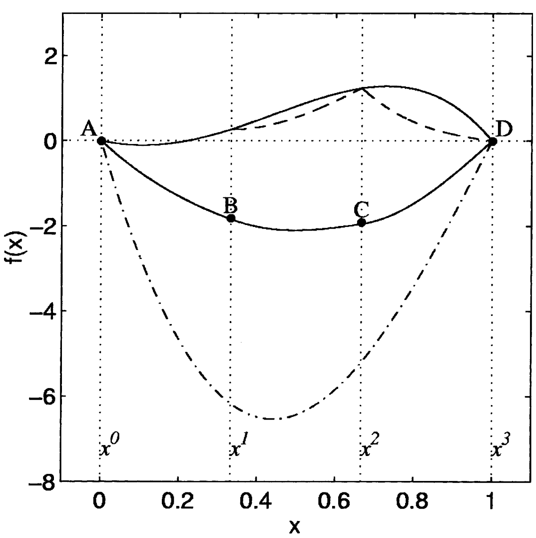

Figure 2. $f(x)$ and convex underestimators: αBB (-·-), αBB over partial domains (– –), piecewise underestimator (–).

The classical αBB underestimator,

$$\phi(x) = f(x) - 29(1 - x)(x - 0)$$

is shown in Figure 2. This underestimator can be improved by partitioning the domain into three subintervals of equal length, $[x^0, x^1], [x^1, x^2], [x^2, x^3]$, where $x^0 = 0, x^1 = \frac{1}{3}, x^2 = \frac{2}{3}$ and $x^3 = 1$ As $f''(x)$ is a monotonically decreasing function, the α values in each interval are derived from the upper bounds on the respective intervals as follows,

$$\alpha^1 = \max\{0, -\tfrac{1}{2}f''(x^1)\} = 0,$$

$$\alpha^2 = \max\{0, -\tfrac{1}{2}f''(x^2)\} = 9\frac{1}{3},$$

$$\alpha^3 = \max\{0, -\tfrac{1}{2}f''(x^3)\} = 29.$$

The classical αBB perturbation functions and underestimators over each of the smaller intervals are depicted in Figures 1 and 2 (dash line). A convex underestimator over the whole interval is constructed by adding a linear function $\beta^i x + \gamma^i$ to the αBB perturbations over each of the subintervals $i = 1, \ldots, 3$. The parameters β^i and γ^i, defining these linear functions are chosen so that the overall perturbation function is smooth and is zero at the end points. These values are calculated using the Equations 7–9. The piecewise quadratic perturbation function, shown in Figure 1 (solid line) is defined as follows:

$$q(x) = q^1(x) \quad \text{for } x \in [0, \tfrac{1}{3}],$$

$$q(x) = q^2(x) \quad \text{for } x \in [\tfrac{1}{3}, \tfrac{2}{3}],$$

$$q(x) = q^3(x) \quad \text{for } x \in [\tfrac{2}{3}, 1],$$

$$q^1(x) = 6.6667x,$$

$$q^2(x) = 9.3333(0.6667 - x)(x - 0.3333) + 3.2221x + 1.0370,$$

$$q^3(x) = 29(1.0 - x)(x - 0.667) - 9.5552x + 9.5551.$$

In Figure 1 the endpoints of the quadratic pieces are labelled A, B, C and D. At the endpoints A and D, the conditions $q^1(x^0) = 0$ and $q^3(x^3) = 0$, respectively, are enforced. Two conditions are enforced at each of the interior points B and C to enforce the smoothness of the piecewise quadratic function. At point B, $q^1(x^1) = q^2(x^1)$ and $\left.\frac{dq^1}{dx}\right|_{x^1} = \left.\frac{dq^2}{dx}\right|_{x^1}$ apply, and at point C, $q^2(x^2) = q^3(x^2)$ and $\left.\frac{dq^2}{dx}\right|_{x^2} = \left.\frac{dq^3}{dx}\right|_{x^2}$ apply. The convex underestimator, which is the difference, $f(x) - q(x)$, is shown in Figure 2 (solid line).

4. Properties of the Underestimator

In this section we prove the smoothness, underestimation, and convexity properties of $\phi(x)$. Smoothness is shown in Proposition 4.1.

PROPOSITION 4.1. *$\phi(x) : \mathbf{x} \ni x \to \mathbb{R}$ is a continously differentiable function.*

Proof. The continuity of $q(x)$ is guaranteed by condition (4), and the continuity of $\frac{\mathrm{d}q(x)}{\mathrm{d}x}$ is guaranteed by condition (6). The smoothness of $\phi(x)$ follows from the smoothness of $f(x)$ and $q(x)$. □

Next we prove that $\phi(x)$ is an underestimator of $f(x)$. Lemma 4.2 shows that $q(x)$ is a concave function. This result is used in Proposition 4.3 to prove that $\phi(x)$ is a underestimator of $f(x)$.

LEMMA 4.2. *If $\alpha_i^k \geqslant 0$ for all $k = 1, \ldots, N_i - 1$, and $i = 1, \ldots, n$, then $q(x)$ is concave over $\mathbf{x}$.*

Proof. By definition $q(x) := \sum_{i=1}^{n} q_i(x_i)$. We will prove the concavity of $q(x)$ by first proving that each $q_i(x_i)$ is concave. On the interval $(x_i^{k-1}, x_i^k), q_i(x_i)$ is C^2 continuous and its second derivative is negative, therefore $q_i(x_i)$ is concave on (x_i^{k-1}, x_i^k). As $q_i^k(x_i)$ is continuous it is also concave on $[x^{k-1}, x^k]$. The derivative of $q_i(x_i)$ is a continuous function as $\frac{\mathrm{d}q_i^k}{\mathrm{d}x_i}\Big|_{x_i^k} = \frac{\mathrm{d}q_i^{k+1}(x_i^k)}{\mathrm{d}x_i}\Big|_{x_i^k}$. Consequently, q_i is a continuous function with an decreasing derivative on $[\underline{x}_i, \bar{x}_i]$ and is thus concave. A sum of concave functions is concave, hence $q(x)$ is concave on $\mathbf{x}$. □

PROPOSITION 4.3. *$\phi(x)$ is an underestimator of $f(x)$, that is $\phi(x) \leqslant f(x)$ for all $x \in \mathbf{x}$.*

Proof. By the convexity of $-q(x)$ and Jensen's Inequality (Hiriart-Urruty and Lemaréchal, 1993),

$$-q(\lambda_1 x^1 + \cdots + \lambda_{n+1} x^{n+1}) \leqslant -\lambda_1 q(x^1) - \cdots - \lambda_{n+1} q(x^{n+1}),$$

when $\lambda_1 + \cdots + \lambda_{n+1} = 1$ and $\lambda_1 \geqslant 0, \ldots, \lambda_{n+1} \geqslant 0$. Carathéodory's Theorem (Rockafeller, 1970, Theorem 17.1) says any $x \in \mathbf{x}$ can be written as a convex combination of $n+1$ vertex points, $x = \lambda_1 x^1 + \cdots + \lambda_{n+1} x^{n+1}$. From conditions (3) and (5), $-q(x) = 0$ for all vertices of the domain $\mathbf{x}$. Therefore,

$$-q(x) \leqslant -\lambda_1 q(x^1) - \cdots - \lambda_{n+1} q(x^{n+1}) \leqslant 0,$$

and $f(x) - q(x) \leqslant f(x)$, as required. □

Finally we show that $\phi(x)$ is convex, using the argument of gradient monotonicity. *Monotonicity* is defined as follows.

DEFINITION (*Hiriart-Urruty and Lemaréchal, 1993*) Let $C \subset \mathbb{R}^n$ be convex. A mapping $F : C \to \mathbb{R}^n$ is said to be monotone on C when for all x and x' in C, $\langle F(x) - F(x'), x - x' \rangle \geqslant 0$ whenever $x \neq x'$.

Proof of the convexity of $\phi(x)$ is based on a generalization of the one dimensional argument used in Lemma 4.2. The following is Theorem IV.4.1.4 from Hiriart-Urruty and Lemaréchal, (1993).

THEOREM 4.4. *Let f be a function differentiable on an open set $\Omega \subset \mathbb{R}^n$, and let C be a convex subset of Ω. Then, f is convex on C if and only if its gradient ∇f is monotone on C.*

Now we can prove the convexity of $\phi(x)$ using Theorem 4.4.

PROPOSITION 4.5. *Let $f : \mathbb{R} \supset \mathbf{x} \to \mathbb{R}$ be a twice continuously differentiable function over $_n\mathbf{x}$. Let $\phi(x) := f(x) - q(x)$ where $q(x)$ is defined by (3)–(6). If $\nabla^2(f(x) - \sum_{i=1} q_i^k(x)) \geqslant 0$ for all $x \in I := [x_1^{k_1-1}, x_1^{k_1}] \times \cdots \times [x_n^{k_n-1}, x_n^{k_n}]$ where $x_i^{k_i} \in \{x_i^1, \ldots, x_i^{N_i-1}\}$, $i = 1, \ldots, n$, then $\phi(x)$ is a convex function on $\mathbf{x}$.*

Proof. Consider a region, I, over which the *piecewise* C^2-continuous function $q(x)$ is C^2-continuous. Let $I := [x_1^{k_1-1}, x_1^{k_1}] \times \cdots \times [x_n^{k_n-1}, x_n^{k_n}]$. As $\nabla^2(f(x) - \sum_{i=1}^{n} q_i^k(x))$ is positive semidefinite on I, $\phi(x)$ is convex on I. From Theorem 4.4 $\langle \nabla\phi(x) - \nabla\phi(x'), x - x' \rangle \geqslant 0$ whenever $x \neq x', x \in I, x' \in I$. Now, consider the case when $x \in I$ and $x' \in I'$ where I and I' are adjacent regions of C^2 continuity, that is $\mathrm{int} I \cap \mathrm{int} I' = \emptyset$ and $I \cap I' \neq \emptyset$. Let $x \in I$, $x' \in I'$ and x^* be such that $x^* \in I \cap I'$ is a point on the line between x and x'. From the convexity of $\phi(x)$ on I',

$$\langle \nabla\phi(x^*) - \nabla\phi(x'), x^* - x' \rangle \geqslant 0,$$

and from the convexity of $\phi(x)$ on I,

$$\langle \nabla\phi(x) - \nabla\phi(x^*), x - x^* \rangle \geqslant 0,$$

therefore,

$$\langle \nabla\phi(x) - \nabla\phi(x^*), x - x^* \rangle + \langle \nabla\phi(x^*) - \nabla\phi(x'), x^* - x' \rangle$$
$$= \langle \nabla\phi(x) - \nabla\phi(x'), x - x' \rangle \geqslant 0.$$

It follows that

$$\langle \nabla\phi(x) - \nabla\phi(x'), x - x' \rangle \geqslant 0.$$

for any x and x' in $\mathbf{x}$ and that ϕ is convex in $\mathbf{x}$.

Illustration 1: Consider the Lennard-Jones potential energy function,

$$f(x) = \frac{1}{x^{12}} - \frac{2}{x^6}$$

in the interval $[\underline{x}, \bar{x}]$ = [0.85, 2.00]. The first term of this function is a convex function and dominates when x is small, while the second term is a concave function which dominates when x is large. The minimum eigenvalue of this function in an interval $[\underline{x}, \bar{x}]$ can be calculated explicitly as follows:

$$\min f'' = \begin{cases} \frac{156}{\bar{x}^{14}} - \frac{84}{\bar{x}^8} & \text{if } \bar{x}\ 1.21707, \\ -7.47810 & \text{if } [\underline{x}, \bar{x}] \ni 1.21707, \\ \frac{156}{\underline{x}^{14}} - \frac{84}{\underline{x}^8} & \text{if } \bar{x} \geqslant 1.21707. \end{cases}$$

The classical αBB underestimator for this function and interval is $f(x) - \frac{7.47810}{2}(\bar{x} - x)(x - \underline{x})$. Bisecting the domain and applying Equations 7–9 we obtain a convex underestimator defined by the parameters in Table l. Partitioning the domain into 16 equal sized subintervals, and applying Equations 7–9 we obtain the convex underestimator $\phi(x)$ with the parameters defining $q(x)$ in Table 2. The potential energy function, the classical αBB underestimator, and the $\phi(x)$ underestimators are shown in Figure 3. In this figure the α spline underestimator based on 2 subregions is denoted, $\phi^{(2)}$, while that based on 16 subregions is denoted, $\phi^{(16)}$.

Illustration 2: As an illustration of the underestimation technique on a function with a domain in $\mathbb{R}^2$, consider the Six-Hump Camelback function (Dixon and Szegö, 1975),

$$f(x_1, x_2) := 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4$$

over the domain $(x_1, x_2) \in [0, 1] \times [0, 1]$, represented in Figure 4. The Hessian matrix of this function is

$$\nabla^2 f(x_1, x_2) = \begin{bmatrix} 8 - 25.2x_1^2 + 10x_1^4 & 1 \\ 1 & -8 + 48x_2^2 \end{bmatrix}.$$

Using the INTPAKX interval arithmetic software (Krämer and Geulig, 2001), an interval Hessian matrix $\mathbf{H}^{[\underline{x}_1,\bar{x}_1]\times[\underline{x}_2,\bar{x}_2]}$ over this domain, is computed as

Table 1. Parameters for two subinterval perturbation for Lennard-Jones function

k	x^k	$\min f''$	α^k	β^k	γ^k
0	0.850				
1	1.425	−7.47810	3.73905	1.62764	−1.38349
2	2.000	−3.84462	1.92231	−1.62764	3.25528

Table 2. Parameters for 16 subinterval perturbation of Lennard-Jones function

k	x^k	min f''	α^k	β^k	γ^k
0	0.850000				
1	0.921875	326.18127	0.00000	1.78326	−1.51577
2	0.993750	81.99112	0.00000	1.78326	−1.51577
3	1.065625	13.55346	0.00000	1.78326	−1.51577
4	1.137500	−4.27629	2.13815	1.62958	−1.35200
5	1.209375	−7.46047	3.73024	1.20779	−0.87222
6	1.281250	−7.47810	3.73905	0.67093	−0.22296
7	1.353125	−6.71098	3.35549	0.16101	0.43038
8	1.425000	−5.21291	2.60645	−0.26750	1.01021
9	1.496875	−3.84462	1.92231	−0.59301	1.47405
10	1.568750	−2.78248	1.39124	−0.83117	1.83055
11	1.640625	−2.00473	1.00236	−1.00321	2.10044
12	1.712500	−1.44791	0.72395	−1.12729	2.30401
13	1.784375	−1.05201	0.52600	−1.21713	2.45786
14	1.856250	−0.77029	0.38515	−1.28262	2.57472
15	1.928125	−0.56887	0.28443	−1.33074	2.66405
16	2.000000	−0.42385	0.21192	−1.36642	2.73284

$$\mathbf{H}^{[0,1]\times[0,1]} = \begin{bmatrix} [-14.03594, 3.82500] & [1.00000, 1.00000] \\ [1.00000, 1.00000] & [-8.00000, 40.00000] \end{bmatrix}.$$

Adjiman et al. (1998b) extended the Gerschgorin Theorem concerning the eigenvalues of real matrices to treat interval matrices. The α parameters for

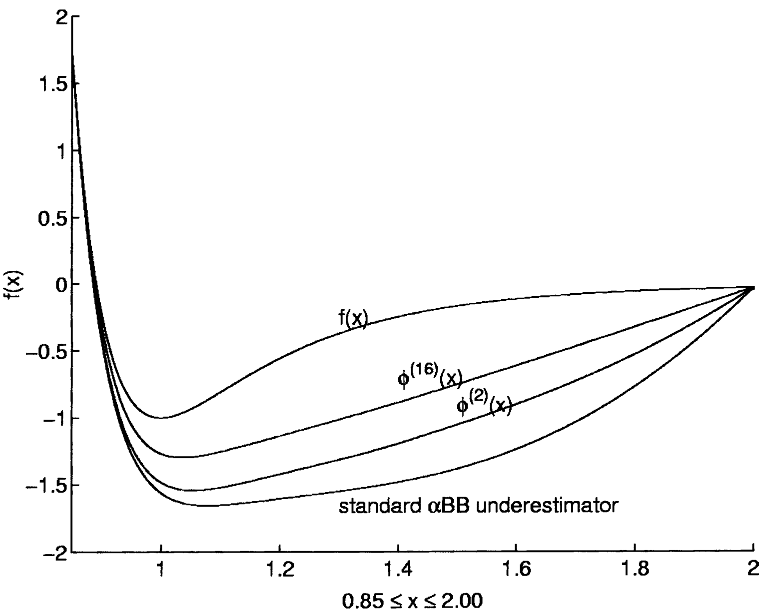

Figure 3. Lennard-Jones potential function and underestimators.

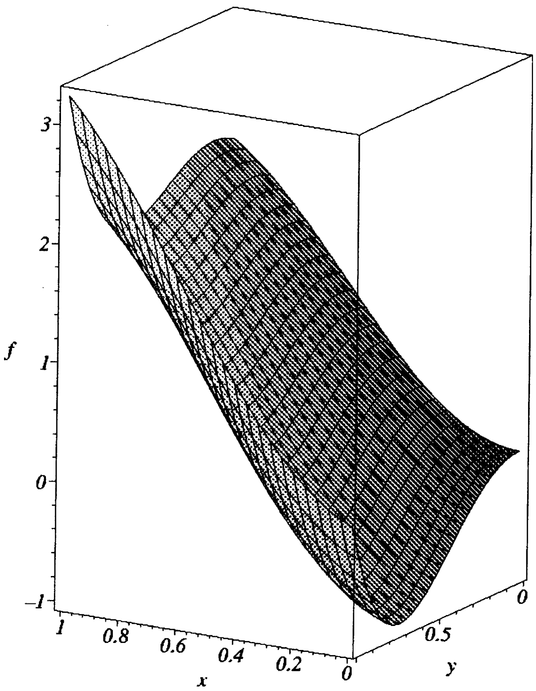

Figure 4. Six-Hump Camelback function.

the classical αBB underestimator are calculated using the formula (Adjiman et al., 1998b)

$$\alpha_i \geqslant -0.5 \min\left\{0, \underline{\mathbf{H}}^{\mathbf{x}}_{ii} - \sum_{j \neq i} \max\{|\underline{\mathbf{H}}^{\mathbf{x}}_{ij}|, |\overline{\mathbf{H}}^{\mathbf{x}}_{ij}|\right\}.$$

The classical αBB underestimator is constructed using the resulting values $\alpha_1 = 8.7875$ and $\alpha_2 = 4.5$.

The αBB convex underestimator can be refined by partitioning the domain into four equal areas by bisection along the x_1 and x_2 axis. The interval Hessians for each of the four regions are

$$\mathbf{H}^{[0,0.5]\times[0,0.5]} = \begin{bmatrix} [1.70000, 8.62500] & [1.00000, 1.00000] \\ [1.00000, 1.00000] & [-8.0000, 4.00000] \end{bmatrix},$$

$$\mathbf{H}^{[0.5,1.0]\times[0,0.5]} = \begin{bmatrix} [-16.57500, 11.7000] & [1.00000, 1.00000] \\ [1.00000, 1.00000] & [-8.00000, 4.00000] \end{bmatrix},$$

$$\mathbf{H}^{[0,0.5]\times[0.5,1]} = \begin{bmatrix} [1.70000, 8.62500] & [1.00000, 1.00000] \\ [1.00000, 1.00000] & [4.00000, 40.00000] \end{bmatrix},$$

$$\mathbf{H}^{[0.5,1]\times[0.5,1]} = \begin{bmatrix} [-16.57500, 11.70000] & [1.00000, 1.00000] \\ [1.00000, 1.00000] & [4.00000, 40.00000] \end{bmatrix}.$$

Sufficiently large α values *for each subregion* may be calculated by applying the formula of Adjiman et al. (1998b) to each of these interval Hessians. The partitioning of the domain into four subregions is illustrated in Figure 5(b). The α values calculated by the interval Gerschgorin formula to be large enough to convexify f in the respective subregions are displayed in this figure.

The underestimation function may be further refined through bisection of the interval $x_1 \in [0.5, 1.0]$ resulting in a partition with six subregions. Figure 5(c) illustrates this partitioning scheme and summarizes the α values calculated using the interval Gerschgorin formula. In Figure 5(d) a further

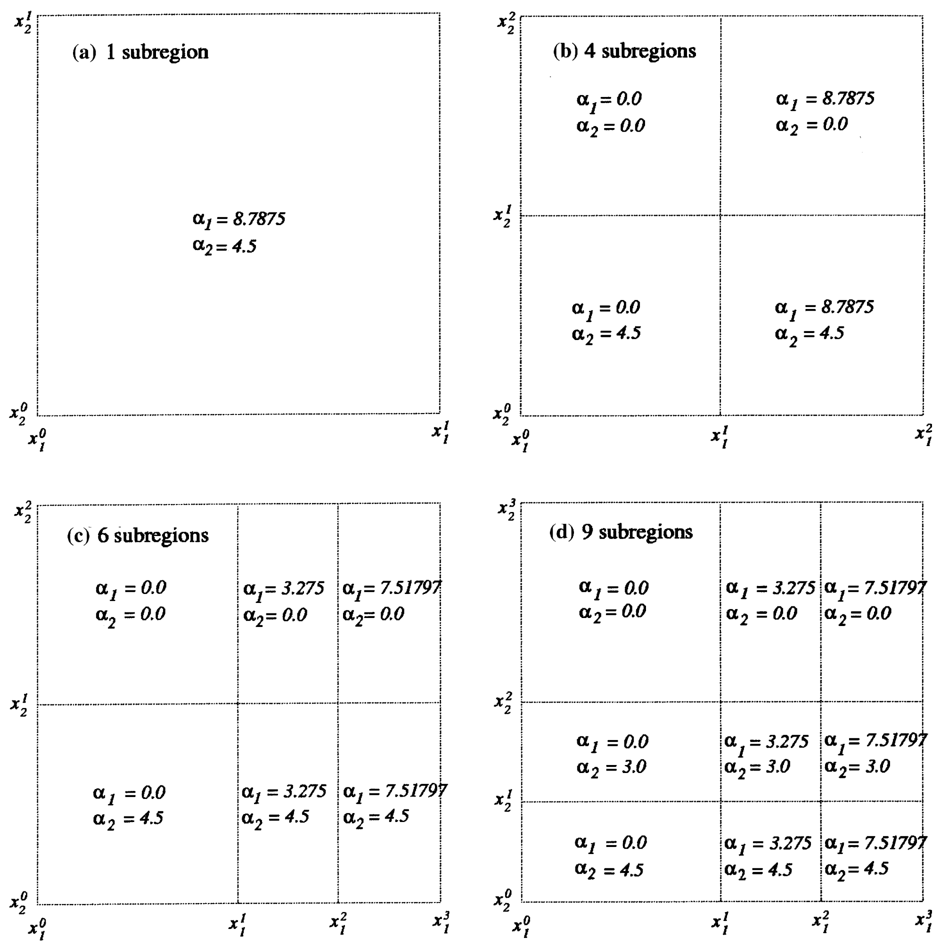

Figure 5. Six-Hump Camelback function α over subregions.

refinement is represented. The parameters for the piecewise C^2 continuous underestimator for each of these partitioning schemes, calculated using Equations 7–9, are summarized in Table 3.

The negative of the α-spline perturbation function, $-q(x)$, over 4, 6, and 9 domains is plotted in Figure 6(a)–(c). The classical αBB perturbation function is shown to significantly overestimate the α-spline functions in each of these figures.

5. Nonconcave Perturbation

Consider a function $f(x)$, such as the Lennard-Jones potential function in which the function is convex in one subdomain and concave in another. In the α spline approach $\phi(x)$ can be convex even if the α values are negative in the regions in which $f(x)$ is strictly convex. In Proposition 4.3 the *underestimation* property is guaranteed by the *concavity* of $q(x)$. The concavity of $q(x)$ is, in turn, a result of the *non-negativity* of the α values. In this section we discuss how the underestimation property of $\phi(x)$ can be maintained when some α values are *negative*.

The underestimation property, $\phi(x) \leqslant f(x)$ for all $x \in \mathbf{x}$, is ensured by the following condition:

$$\min_{x \in \mathbf{x}} q(x) \geqslant 0.$$

Instead of solving minimization problems, the key idea is to adjust the α's to prevent the creation of local minima at any nonvertex point in $\mathbf{x}$ by prohibiting the occurrence of *stationary points* on convex regions of the perturbation function. This is illustrated in Figure 7. In Figure 7(a) a con-

Table 3. Parameters defining the piecewise αBB underestimators for the Six-Hump Camelback function with 4, 6 and 9 subregions

k	x_1^k	α_1^k	β_1^k	γ_1^k	x_2^k	α_2^k	β_2^k	γ_2^k
Four subregions								
0	0.0				0.0			
1	0.5	0.0000	1.125	0.000	0.5	4.5000	1.94688	0.00000
2	1.0	8.7875	−1.125	1.125	1.0	0.0000	−1.94688	1.94688
Six subregions								
0	0.00				0.0			
1	0.50	0.00000	1.08394	0.00000	0.5	4.50000	1.94688	0.00000
2	0.75	3.27500	0.26519	0.40937	1.0	0.00000	−1.94688	1.94688
3	1.00	7.51797	−2.43306	2.43306				
Nine subregions								
0	0.00				0.0			
1	0.50	0.00000	1.08394	0.00000	0.25	4.50000	1.78125	0.00000
2	0.75	3.27500	0.26519	0.40937	0.5	3.00000	−0.09375	0.46875
3	1.00	7.51797	−2.43306	2.43306	1.0	0.00000	−0.84375	0.84375

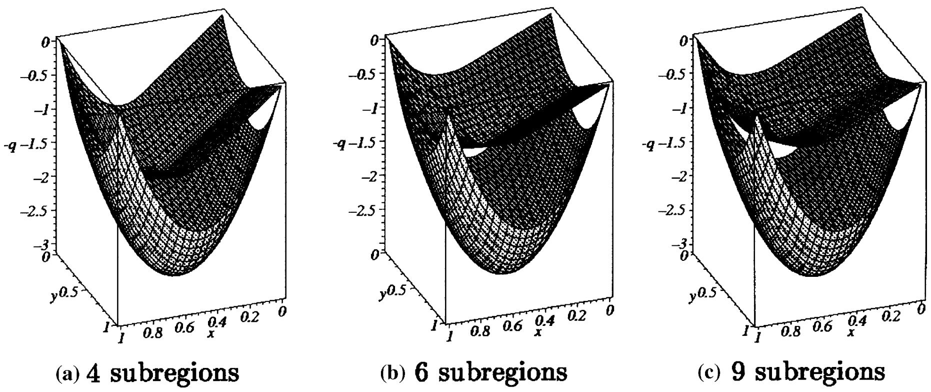

Figure 6. Six-Hump Camelback function: αBB and piecewise αBB perturbations with 4, 6 and 9 subregions.

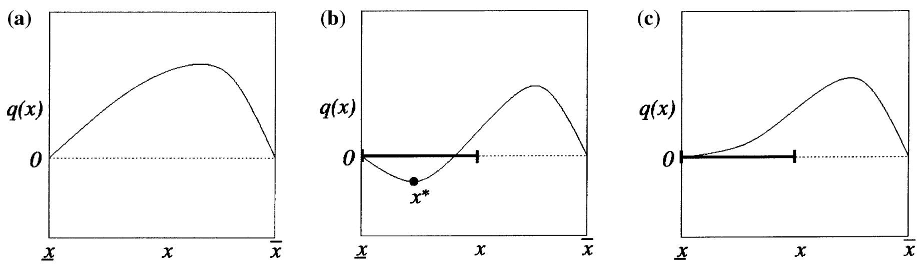

Figure 7. (a) Concave, (b) nonconcave, and (c) nonnegative nonconcave perturbation functions.

cave perturbation function is depicted. The nonnegativity of this function follows from its concavity. In Figure 7(b) a perturbation function is shown which is *convex* over the domain marked with a bold line.

The point x^* is a *stationary point* of q in this convex region and we note that $q(x^*)$ is *negative*. In Figure 7(c) the perturbation function is again *convex* over the marked region but there is no stationary point in this region. This function is nonnegative over the entire domain $[\underline{x}, \overline{x}]$. Using this idea, a tight convex underestimator is derived by starting with $q(x)$, with nonnegative α values as defined in Section 2, and making the zero α's negative one at a time, while maintaining the convexity of $\phi(x)$ and avoiding the generation of stationary points on the convex portions of q.

The remainder of this section is structured as follows. First, the dependence of the parameters β on the α parameters is derived. Next, stationary conditions for $q(x)$ are derived and used to define conditions on the α's which guarantee the absence of stationary points on the convex portions of $q(x)$. This leads to a method that is effective when the convex regions lie at extrema of the domain. Finally we consider a technique for generating tight convex relaxations for functions which have convex regions which are not at the domain extrema.

For the rest of this section we will assume that $f : \mathbf{x} \to \mathbb{R}$ is a univariate function, $\mathbf{x} = [\underline{x}, \overline{x}] \subset \mathbb{R}$. The separable structure of the α spline function allows the techniques developed here to be applied to the multivariate case.

5.1. FUNCTIONAL DEPENDENCE OF β ON α

Note that the β and γ parameters defining $q(x)$ are functions of the α's and the endpoints, $x^0, \ldots, x^N$. The following formula, derived from Equations 7–9, is an expression for β^k in terms of $\alpha^1, \ldots, \alpha^N$

$$\beta^k = \frac{1}{x^N - x^0}\sum_{j=1}^{k-1}(-\alpha^j(x^j - x^{j-1})(x^j - x^0) - \alpha^{j+1}(x^{j+1} - x^j)(x^j - x^0)) + \frac{1}{x^N - x^0}\sum_{j=k}^{N-1}(-\alpha^j(x^j - x^{j-1})(x^j - x^N) - \alpha^{j+1}(x^{j+1} - x^j)(x^j - x^N)).$$

Suppose that having calculated $\beta \in \mathbb{R}^N$ for some given $\alpha \in \mathbb{R}^N$, we wish to modify some element α^j. Below, we derive formulae that may be used to update the β's following such an α update. Under the substitution $\alpha^j \to \tilde{\alpha}^j$ the elements $\tilde{\beta}^1, \ldots, \tilde{\beta}^N$ that satisfy Equations 7–9 may be expressed in terms of $\beta^1, \ldots, \beta^N, \alpha^j$ and $\tilde{\alpha}^j$ using the update formulae,

$$\begin{aligned}\tilde{\beta}^k - \beta^k &= \frac{1}{x^N - x^0}(\alpha^j - \tilde{\alpha}^j)(x^j - x^{j-1})(x^{j-1} - x^0) \\ &\quad + \frac{1}{x^N - x^0}(\alpha^j - \tilde{\alpha}^j)(x^j - x^{j-1})(x^j - x^0) \\ &= \frac{1}{x^N - x^0}(\alpha^j - \tilde{\alpha}^j)(x^j - x^{j-1})(x^{j-1} + x^j - 2x^0) \quad \text{if} \quad j < k, \end{aligned} \tag{10}$$

$$\begin{aligned}\tilde{\beta}^k - \beta^k &= \frac{1}{x^N - x^0}(\alpha^j - \tilde{\alpha}^j)(x^j - x^{j-1})(x^{j-1} - x^0) \\ &\quad + \frac{1}{x^N - x^0}(\alpha^j - \tilde{\alpha}^j)(x^j - x^{j-1})(x^j - x^N) \\ &= \frac{1}{x^N - x^0}(\alpha^j - \tilde{\alpha}^j)(x^j - x^{j-1})(x^{j-1} + x^j - x^0 - x^N) \quad \text{if} \quad j = k, \end{aligned} \tag{11}$$

$$\begin{aligned}\tilde{\beta}^k - \beta^k &= \frac{1}{x^N - x^0}(\alpha^j - \tilde{\alpha}^j)(x^j - x^{j-1})(x^{j-1} - x^N) \\ &\quad + \frac{1}{x^N - x^0}(\alpha^j - \tilde{\alpha}^j)(x^j - x^{j-1})(x^j - x^N) \\ &= \frac{1}{x^N - x^0}(\alpha^j - \tilde{\alpha}^j)(x^j - x^{j-1})(x^{j-1} + x^j - 2x^N) \quad \text{if} \quad j > k. \end{aligned} \tag{12}$$

5.2. PERTURBATION FUNCTION STATIONARY POINTS

A stationary point x^* of the function $q : \mathbb{R} \to \mathbb{R}$ is one that satisfies

$$\left.\frac{dq}{dx}\right|_{x^*} = 0$$

or

$$\alpha^k(x^k + x^{k-1} - 2x^*) + \beta^k = 0$$

in some interval, $x^* \in [x^{k-1}, x^k]$. From this we see that $x^* = \frac{1}{2}(x^k + x^{k-1} + \beta^k/\alpha^k)$ if $x^{k-1} \leqslant x^* \leqslant x^k$ for some $k \in \{1, \ldots, N\}$. It follows that an interval k contains no stationary point if either $\frac{1}{2}(x^k + x^{k-1} + \beta^k/\alpha^k) > x^k$ or $\frac{1}{2}(x^k + x^{k-1} + \beta^k/\alpha^k) < x^{k-1}$.

The following three Lemmas 5.1–5.3, provide conditions on α^j that guarantee the absence of a stationary point in an interval $[x^{k-1}, x^k]$. There are three cases, $j < k$, $j = k$, and $j > k$, which are treated separately in the respective lemmas.

LEMMA 5.1. *Consider two intervals* $[x^{j-1}, x^j]$ *and* $[x^{k-1}, x^k]$ *where* $j < k$. *Let the sequence of* α *values defining* $q^k(x)$ *be*

$$\{\alpha^1, \ldots, \alpha^j, \ldots, \alpha^k, \ldots, \alpha^{N-1}\},$$

where $\alpha^k < 0$. Let $\tilde{q}^k(x)$ *be the function defined by the sequence of* α *values*

$$\{\alpha^1, \ldots, \tilde{\alpha}^j, \ldots, \alpha^k, \ldots, \alpha^{N-1}\},$$

where $\tilde{\alpha}^j < 0$. *There exists no stationary point of* $\tilde{q}^k(x)$ *on the interval* $[x^{k-1}, x^k]$ *if either of the following bounds on* $\tilde{\alpha}^j$ *hold*:

$$\tilde{\alpha}^j > \frac{(x^N - x^0)(-\alpha^k(x^k - x^{k-1}) + \beta^k) + \alpha^j(x^j - x^{j-1})(x^{j-1} + x^j - 2x^0)}{(x^j - x^{j-1})(x^j + x^{j-1} - 2x^0)}$$

or

$$\tilde{\alpha}^j < \frac{(x^N - x^0)(\alpha^k(x^k - x^{k-1}) + \beta^k) + \alpha^j(x^j - x^{j-1})(x^{j-1} + x^j - 2x^0)}{(x^j - x^{j-1})(x^j + x^{j-1} - 2x^0)}.$$

Proof. *Lower bound on* $\tilde{\alpha}^j$: Let x^* be a stationary point of $\tilde{q}^k(x)$. Suppose $x^* = \frac{1}{2}(x^k + x^{k-1} + \frac{\tilde{\beta}^k}{\alpha^k}) > x^k$ then

$$-x^k + x^{k-1} + \frac{\tilde{\beta}^k}{\alpha^k} > 0.$$

α^k is strictly negative, therefore

$$\alpha^k(x^k - x^{k-1}) - \tilde{\beta}^k > 0.$$

Using (10) to express $\tilde{\beta}^k$ as a function of $\tilde{\alpha}^j$ we get,

$$\alpha^k(x^k - x^{k-1}) - \beta^k - \frac{1}{x^N - x^0}(\alpha^j - \tilde{\alpha}^j)(x^j - x^{j-1})(x^{j-1} + x^j - 2x^0) > 0$$

.

As $(x^N - x^0), (x^j - x^{j-1})$, and $(x^j + x^{j-1} - 2x^0)$ are strictly positive we can derive an upper bound on $\tilde{\alpha}^j$

$$\tilde{\alpha}^j > \frac{(x^N - x^0)(-\alpha^k(x^k - x^{k-1}) + \beta^k) + \alpha^j(x^j - x^{j-1})(x^{j-1} + x^j - 2x^0)}{(x^j - x^{j-1})(x^j + x^{j-1} - 2x^0)}.$$

Upper bound on $\tilde{\alpha}^j$*:* suppose $x^* = \frac{1}{2}(x^k + x^{k-1} + \frac{\tilde{\beta}^k}{\alpha^k}) < x^{k-1}$ then

$$x^k - x^{k-1} + \frac{\tilde{\beta}^k}{\alpha^k} < 0.$$

α^k is strictly negative, therefore

$$\alpha^k(x^k - x^{k-1}) + \tilde{\beta}^k > 0.$$

Using (10) to express $\tilde{\beta}^k$ as a function of $\tilde{\alpha}^j$ we get,

$$\alpha^k(x^k - x^{k-1}) + \beta^k + \frac{1}{x^N - x^0}(\alpha^j - \tilde{\alpha}^j)(x^j - x^{j-1})(x^{j-1} + x^j - 2x^0) > 0.$$

As $(x^N - x^0), (x^j - x^{j-1})$, and $(x^j + x^{j-1} - 2x^0)$ are strictly positive we can derive an upper bound on $\tilde{\alpha}^j$

$$\tilde{\alpha}^j < \frac{(x^N - x^0)(\alpha^k(x^k - x^{k-1}) + \beta^k) + \alpha^j(x^j - x^{j-1})(x^{j-1} + x^j - 2x^0)}{(x^j - x^{j-1})(x^j + x^{j-1} - 2x^0)}$$

LEMMA 5.2. *Consider an interval* $[x^{k-1}, x^k]$*. Let* $\{\alpha^1, \alpha^2, \ldots, \alpha^{N-1}\}$ *be the sequence of* α *values determining* $q^k(x)$*. Let* $\tilde{q}^k(x)$ *be the function defined by the sequence of* α *values* $\{\alpha^1, \ldots, \alpha^{k-1}, \tilde{\alpha}^k, \alpha^{k+1}, \ldots, \alpha^{N-1}\}$ *where* $\tilde{\alpha}^k < 0$*. A stationary point of* $\tilde{q}(x)$ *does not exist on the interval* $[x^{k-1}, x^k]$ *if either of the following conditions hold:*

$$\tilde{\alpha}^k > \frac{\zeta}{(x^k - x^{k-1})(x^k + x^{k-1} - 2x^0)} \quad \text{if } \zeta \leqslant 0,$$
$$\tilde{\alpha}^k > \frac{\zeta}{(x^k - x^{k-1})(x^k + x^{k-1} - 2x^N)} \quad \text{if } \zeta > 0, \tag{13}$$

where $\zeta = \beta^k(x^N - x^0) + \alpha^k(x^k - x^{k-1})(x^{k-1} + x^k - x^0 - x^N)$.

Proof. $x^* > x^k$: As $\tilde{q}^k(x)$ is a strictly convex quadratic function, it can have at most one stationary point x^*. Suppose $x^* = \frac{1}{2}(x^k + x^{k-1} + \frac{\tilde{\beta}^k}{\alpha^k}) > x^k$ then

$$-x^k + x^{k-1} + \frac{\tilde{\beta}^k}{\tilde{\alpha}^k} > 0.$$

$\tilde{\alpha}^k$ is strictly negative, therefore

$$\tilde{\alpha}^k(x^k - x^{k-1}) - \tilde{\beta}^k > 0.$$

Using (11) to express $\tilde{\beta}^k$ as a function of $\tilde{\alpha}^k$ we get,

$$\tilde{\alpha}^k(x^k - x^{k-1}) - \beta^k - \frac{1}{x^N - x^0}(\alpha^k - \tilde{\alpha}^k)(x^k - x^{k-1}) \times (x^{k-1} + x^k - x^0 - x^N) > 0.$$

As $(x^N - x^0), (x^k - x^{k-1})$, and $(x^k + x^{k-1} - 2x^0)$ are strictly positive we can derive a lower bound on $\tilde{\alpha}^k$

$$\tilde{\alpha}^k > \frac{(x^N - x^0)(\beta^k) + \alpha^k(x^k - x^{k-1})(x^{k-1} + x^k - x^0 - x^N)}{(x^k - x^{k-1})(x^k + x^{k-1} - 2x^0)}.$$

$x^* < x^{k-1}$: Suppose $x^* = \frac{1}{2}(x^k + x^{k-1} + \frac{\tilde{\beta}^k}{\tilde{\alpha}^k}) < x^{k-1}$ then

$$x^k - x^{k-1} + \frac{\tilde{\beta}^k}{\tilde{\alpha}^k} < 0.$$

$\tilde{\alpha}^k$ is strictly negative, therefore

$$\tilde{\alpha}^k(x^k - x^{k-1}) + \tilde{\beta}^k > 0.$$

Using (11) to express $\tilde{\beta}^k$ as a function of $\tilde{\alpha}^k$ we get,

$$\tilde{\alpha}^k(x^k - x^{k-1}) + \beta^k + \frac{1}{x^N - x^0}(\alpha^k - \tilde{\alpha}^k)(x^k - x^{k-1}) \times (x^{k-1} + x^k - x^0 - x^N) > 0.$$

As $(x^N - x^0), (x^k - x^{k-1})$, and $(2x^N - x^k - x^{k-1})$ are strictly positive we can derive a lower bound on $\tilde{\alpha}^j$

$$\tilde{\alpha}^k > \frac{-(x^N - x^0)\beta^k - \alpha^k(x^k - x^{k-1})(x^{k-1} + x^k - x^0 - x^N)}{(x^k - x^{k-1})(2x^N - x^k - x^{k-1})}. \qquad \square$$

LEMMA 5.3. *Consider two intervals* $[x^{j-1}, x^j]$ *and* $[x^k, x^{k-1}]$ *where* $j > k$. *Let* $\alpha^k < 0$, *and* $\{\alpha^1, \ldots, \alpha^k, \ldots, \alpha^j, \ldots, \alpha^{N-1}\}$ *be the sequence of* α *values determining* $q^k(x)$. *Let* $\tilde{q}^k(x)$ *be the function defined by the sequence of* α *values* $\{\alpha^1, \ldots, \alpha^k, \ldots, \tilde{\alpha}^j, \ldots, \alpha^{N-1}\}$ *where* $\tilde{\alpha}^j < 0$. *A stationary point of* $\tilde{q}^k(x)$ *does not exist on the interval* $[x^{k-1}, x^k]$ *if either of the following bounds on* $\tilde{\alpha}^j$ *hold*:

$$\tilde{\alpha}^j > \frac{(x^N - x^0)(\alpha^k(x^k - x^{k-1}) + \beta^k) + \alpha^j(x^j - x^{j-1})(x^{j-1} + x^j - 2x^N)}{(x^j - x^{j-1})(x^j + x^{j-1} - 2x^N)},$$

$$\tilde{\alpha}^j < -\frac{(x^N - x^0)(\alpha^k(x^k - x^{k-1}) - \beta^k) + \alpha^j(x^j - x^{j-1})(x^{j-1} + x^j - 2x^N)}{(x^j - x^{j-1})(x^j + x^{j-1} - 2x^N)}.$$

Proof. Lower bound on $\tilde{\alpha}^j$: Suppose $x^* = \frac{1}{2}(x^k + x^{k-1} + \frac{\tilde{\beta}^k}{\alpha^k}) < x^{k-1}$ then

$$x^k - x^{k-1} + \frac{\tilde{\beta}^k}{\alpha^k} < 0.$$

α^k is strictly negative, therefore

$$\alpha^k\left(x^k - x^{k-1}\right) + \tilde{\beta}^k > 0.$$

Using (12) to express $\tilde{\beta}^k$ as a function of $\tilde{\alpha}^j$ we get,

$$\alpha^k(x^k - x^{k-1}) + \beta^k + \frac{1}{x^N - x^0}(\alpha^j - \tilde{\alpha}^j)(x^j - x^{j-1})(x^{j-1} + x^j - 2x^N) > 0.$$

As $(x^N - x^0), (x^j - x^{j-1})$, and $(2x^N - x^j - x^{j-1})$ are strictly positive we can derive a lower bound on $\tilde{\alpha}^j$

$$\tilde{\alpha}^j > \frac{(x^N - x^0)(\alpha^k(x^k - x^{k-1}) + \beta^k) + \alpha^j(x^j - x^{j-1})(x^{j-1} + x^j - 2x^N)}{(x^j - x^{j-1})(x^j + x^{j-1} - 2x^N)}.$$

Upper bound on $\tilde{\alpha}^j$: As $\tilde{q}^k(x)$ is a strictly concave quadratic function, it can have at most one stationary point x^*. Suppose $x^* = \frac{1}{2}(x^k + x^{k-1} + \frac{\tilde{\beta}^k}{\alpha^k}) > x^k$ then

$$-x^k + x^{k-1} + \frac{\tilde{\beta}^k}{\alpha^k} > 0.$$

α^k is strictly negative, therefore

$$\alpha^k(x^k - x^{k-1}) - \tilde{\beta}^k > 0.$$

Using (12) to express $\tilde{\beta}^k$ as a function of $\tilde{\alpha}^j$ we get,

$$\alpha^k(x^k - x^{k-1}) - \beta^k - \frac{1}{x^N - x^0}(\alpha^j - \tilde{\alpha}^j)(x^j - x^{j-1})(x^{j-1} + x^j - 2x^N) > 0.$$

As $(x^N - x^0), (x^j - x^{j-1})$, and $(2x^N - x^j - x^{j-1})$ are strictly positive we can derive a upper bound on $\tilde{\alpha}^j$

$$\tilde{\alpha}^j < -\frac{(x^N - x^0)(\alpha^k(x^k - x^{k-1}) - \beta^k) + \alpha^j(x^j - x^{j-1})(x^{j-1} + x^j - 2x^N)}{(x^j - x^{j-1})(x^j + x^{j-1} - 2x^N)}.$$

□

5.3. POSITIVITY OF THE PERTURBATION FUNCTION

When $q(x)$ is concave on a set of intervals and is guaranteed to have no stationary point on the remainder of the intervals, $q(x)$ is monotonically nondecreasing between x^0 and a global maximum x^* and monotonically nonincreasing between x^* and x^N. This assertion is proven in Lemma 5.4 and used in Proposition 5.5 to show the positivity of $q(x)$ under the aforementioned conditions.

LEMMA 5.4. *Let* $q(x)$ *be defined by* (7)–(9) where the α *values are such that for each* $k \in \{1, \ldots, N-1\}, \alpha^k \geq 0$ *or* $q^k(x)$ *has no stationary point in* $[x^{k-1}, x^k]$. *If* $x' \in [x^k, x^{k+1}]$ *and* $\frac{dq}{dx}\big|_{x^k} \leqslant 0$ *then* $q(x) \leqslant q(x')$ *for all* $x \in [x', x^N]$. *If* $x' \in [x^{k-1}, x^k]$ *and* $\frac{dq}{dx}\big|_{x^k} \geq 0$ *then* $q(x) \leqslant q(x')$ *for all* $x \in [x^0, x']$.

Proof. $x \geqslant x^k$: Let $x \geqslant x'$ be in the interval $[x^k, x^{k+1}]$. If α^{k+1} is positive, $\frac{dq^{k+1}}{dx}$ is negative for all $x \in [x^k, x^{k+1}]$, and $q^{k+1}(x) \leqslant q^{k+1}(x')$ for all $x \in [x^k, x^{k+1}]$.

If α^{k+1} is strictly negative, $\frac{dq^{k+1}}{dx} < 0$ for all $x \in [x^k, x^{k+1}]$by assumption, therefore $q^{k+1}(x) < q^{k+1}(x')$ for all $x \in [x^k, x^{k+1}]$. In either case $\left.\frac{dq^{k+1}}{dx}\right|_{x^{k+1}} \leqslant 0$ and $q^{k+1}(x^{k+1}) \leqslant q^{k+1}(x^k)$. From the continuity properties of $q(x)$, $q^k(x^k) = q^{k+1}(x^k)$ and $\left.\frac{dq^k}{dx}\right|_{x^k} = \left.\frac{dq^{k+1}}{dx}\right|_{x^k}$. Therefore if $\left.\frac{dq}{dx}\right|_{x^k} \leqslant 0$ then $\left.\frac{dq}{dx}\right|_{x^{k+1}} \leqslant 0$ and by induction $q(x) \leqslant q(x')$ for $x \in [x', x^N]$.

$x \leqslant x^k$: Let $x \leqslant x'$ be in the interval $[x^{k-1}, x^k]$. If α^k is positive, $\frac{dq^k}{dx}$ is positive for all $x \in [x^{k-1}, x^k]$, and $q^k(x) \leqslant q^k(x')$ for all $x \in [x^{k-1}, x']$. If α^k is strictly negative, $\frac{dq^k}{dx} > 0$ for all $x \in [x^{k-1}, x^k]$ by assumption, therefore $q^k(x) \leqslant q^k(x')$ for all $x \in [x^{k-1}, x']$. In either case $\left.\frac{dq}{dx}\right|_{x^{k-1}} \geqslant 0$ and $q^k(x^{k-1}) \leqslant q^k(x')$. Therefore if $\left.\frac{dq}{dx}\right|_{x^k} \geqslant 0$ then $\left.\frac{dq}{dx}\right|_{x^{k-1}} \geqslant 0$ and by induction $q(x) \leqslant q(x')$ for $x \in [x^0, x']$.

PROPOSITION 5.5. *Let $q(x)$ be defined by Equations 7–9 where the α's are such that $q(x)$ cannot have a stationary point in $[x^{k-1}, x^k]$ unless $\alpha^k \geqslant 0$. Under these assumptions $q(x) \geqslant 0$ for all $x \in [x^0, x^N]$.*

Proof. From $q(x^0) = q(x^N) = 0$ and the Mean Value Theorem $\left.\frac{dq}{dx}\right|_{x^*} = 0$ for some $x^* \in (x^0, x^N)$. Let the stationary point x^* lie in the interval $[x^{k-1}, x^k]$. As $q^k(x)$ is assumed to have no stationary points if α^k is strictly negative, α^k must be positive, therefore $q(x)$ is concave over the interval $[x^{k-1}, x^k]$ and x^* is a global maximum of $q(x)$ on this interval. Furthermore, $\left.\frac{dq^k}{dx}\right|_{x^{k-1}} \geqslant 0$ and $\left.\frac{dq^k}{dx}\right|_{x^k} \leqslant 0$. From Lemma 5.4 $q(x) \leqslant q(x')$ for $x \geqslant x' \geqslant x^k$ and $q(x) \leqslant q(x')$ for $x \leqslant x' \leqslant x^{k-1}$. So $q(x)$ is nondecreasing on $[x^0, x^*]$, and nonincreasing on $[x^*, x^N]$ while $q(x^0) = q(x^N) = 0$. Therefore $q(x) \geqslant 0$ for all $x \in [x^0, x^N]$.

5.4. ILLUSTRATIONS OF THE NONCONCAVE PERTURBATION FUNCTION

Illustration 3: This illustration demonstrates the strengthening of an underestimation function through the use of negative α values. Consider the cubic funtion $f(x) = x^3$ on the domain $x \in [-1, 1]$. The second derivative of this function is $\frac{d^2 f}{dx^2} = 6x$. In any interval, $[x^{k-1}, x^k]$, the second derivative lies in the interval $[6x^{k-1}, 6x^k]$. Let the domain be partitioned into eight equal intervals defined by the end points,

$$\{x^0, \ldots, x^8\} = \{-1.0, -0.75, -0.5, -0.25, 0.0, 0.25, 0.5, 0.75, 1.0\}.$$

A valid underestimation function can be derived by setting

$$\alpha^k = \frac{1}{2}(\max\{0, -6x^{k-1}\}),$$
$$\{\alpha^1, \ldots, \alpha^8\} = \{3.0, 2.25, 1.5, 0.75, 0, 0, 0, 0\}.$$

The β and γ vectors are calculated using (7)–(9). Now, we will improve the underestimation by using negative α's. α^5 cannot be decreased as the lower bound of $\frac{d^2f}{dx^2}$ is 0 in the interval $[x^4, x^5] = [0, 0.25]$. The lower bound of $\frac{d^2f}{dx^2}$ in the interval $[x^5, x^6] = [0.25, 0.50]$ is 1.5, therefore the *convexity* of $f(x) - q(x)$ may be maintained if α^6 is decreased to $1.5/2 = -0.75$. However, to ensure that *no stationary points* exist in $[x^5, x^6]$ conditon (13) is enforced. First ζ is calculated:

$$\zeta = \beta^6(x^8 - x^0) + \alpha^6(x^6 - x^5)(x^5 + x^6 - x^0 - x^8) = -1.406 < 0.$$

ζ is negative, so the following inequality applies:

$$\tilde{\alpha}^6 > \frac{\zeta}{(x^6 - x^5)(x^6 + x^5 - 2x^0)} = -2.045.$$

Setting $\alpha^6 = \max\{-0.75, -3.282\} = -0.75$, and recalculating β and γ using (7)–(9) an improved convex underestimation function is defined. In the interval $[x^6, x^7] = [0.5, 0.75]$, the lower bound of $\frac{d^2f}{dx^2}$ is 3.0, therefore α^7 may be decreased to -1.50 without making $q(x)$ convex. To ensure that no stationary points exist in $[x^6, x^7]$ condition (13) is enforced. Now, $\zeta = \beta^7(x^8 - x^0) + \alpha^7(x^7 - x^6)(x^6 + x^7 - x^0 - x^8) = -0.891 < 0$ so the following inequality applies:

$$\tilde{\alpha}^7 > \frac{\zeta}{(x^7 - x^6)(x^7 + x^6 - 2x^0)} = -1.096.$$

We set $\alpha^7 = \max\{-1.500, -1.096\} = -1.096$ and recalculated the β's and γ's. In the interval $[x^7, x^8] = [0.75, 1.0]$, the lower bound of $\frac{d^2f}{dx^2}$ is 4.5, therefore the concavity of $q(x)$ may be maintained even if α^8 is decreased to -2.25. To ensure that no stationary points exist in $[x^7, x^8]$ (13) is enforced. Now, $\zeta = \beta^8(x^8 - x^0) + \alpha^8(x^8 - x^7)(x^7 + x^8 - x^0 - x^8) = 0$ so the following inequality applies:

$$\tilde{\alpha}^8 > \frac{\zeta}{(x^8 - x^7)(x^8 + x^7 - 2x^0)} = 0.$$

So α^8 cannot be decreased and no further modification can be made. Figure 8 illustrates the change in $q(x)$ as a result of the modification of α^6 and α^7, and Figure 9 depicts the improvement in the underestimation function $x^3 - q(x)$.

Illustration 1 continued: Here we consider the convex underestimation of the Lennard-Jones potential energy function discussed in Illustration 1. The parameters for the α-spline function are summarized in Table 4. A negative α value has been assigned to two of the three regions in which the second derivative is strictly positive. In Figure 10 the underestimator with

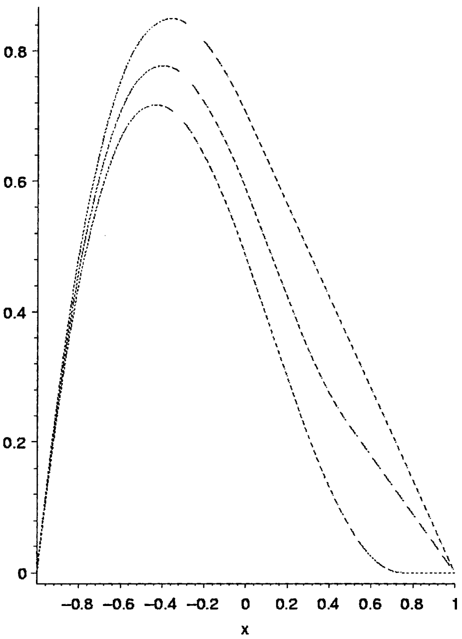

Figure 8. Convex underestimation of x^3 perturbation $q(x)$ with (a) positive α's, (b) $\alpha^6 < 0$, (c) $\alpha^6 < 0$, $\alpha^7 < 0$.

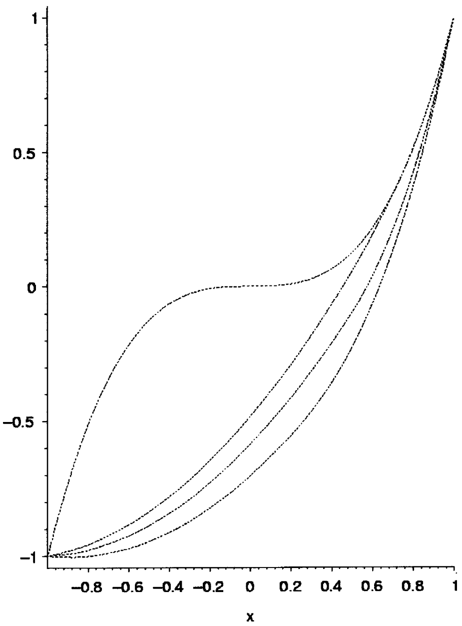

Figure 9. Convex underestimation of x^3:underestimator $x^3 - q(x)$ with (a) postitive α's, (b) $\alpha^6 < 0$, (c) $\alpha^6 < 0$, $\alpha^7 < 0$.

Table 4. Parameters defining $q(x)$ with negative α's for Lennard-Jones potential

k	x^k	min f''	α^k	β^k	γ^k
0	0.850000				
1	0.921875	326.18127	0.00000	0.00000	0.00000
2	0.993750	81.99112	−7.37920	0.53038	−0.48894
3	1.065625	13.55346	−6.77673	1.54784	−1.50004
4	1.137500	−4.27629	2.13815	1.88124	−1.85532
5	1.209375	−7.46047	3.73024	1.45945	−1.37553
6	1.281250	−7.47810	3.73905	0.92259	−0.72627
7	1.353125	−6.71098	3.35549	0.41267	−0.07294
8	1.425000	−5.21291	2.60645	−0.01584	0.50689
9	1.496875	−3.84462	1.92230	−0.34135	0.97074
10	1.568750	−2.78248	1.39124	−0.57951	1.32724
11	1.640625	−2.00473	1.00236	−0.75155	1.59713
12	1.712500	−1.44791	0.72395	−0.87563	1.80069
13	1.784375	−1.05201	0.52600	−0.96547	1.95454
14	1.856250	−0.77029	0.38515	−1.03096	2.07140
15	1.928125	−0.56887	0.28443	−1.07909	2.16074
16	2.000000	−0.42385	0.21192	−1.11476	2.22952

negative α's, marked as $\phi^-(x)$, is shown with the potential energy function and $\phi^+(x)$, the underestimator with negative α's.

This underestimator can be further tightened by refining the partition, particularly in the convex region.

Illustration 2 continued: Here we reconsider the underestimation of the function in Illustration 2 using negative α parameters. Partitioning the

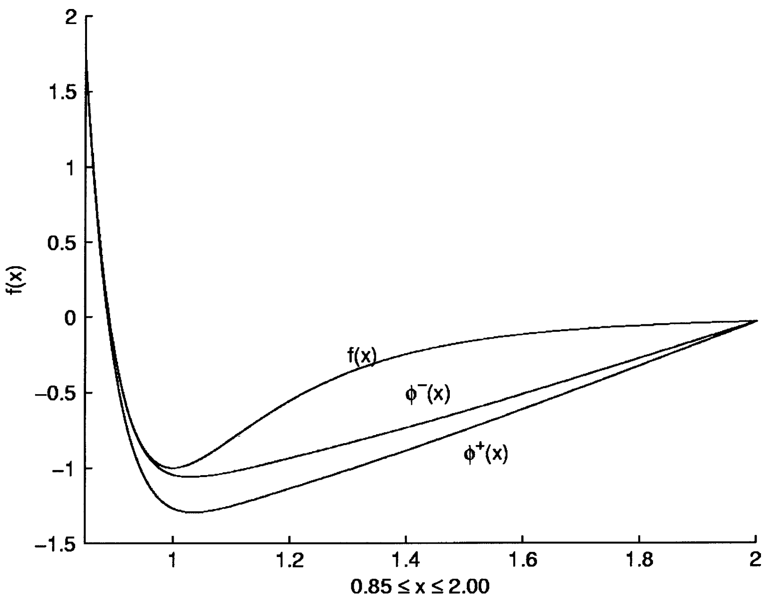

Figure 10. Lennard-Jones convex underestimators with concave and nonconcave perturbations.

domain into nine regions as before, this time applying the α update procedure to both q_1 and q_2 we obtain the parameters in Table 5. In this table $\underline{\lambda}_i := \underline{\mathbf{H}}^{\mathbf{x}}_{ii} - \sum_{j \neq i} \max\left\{|\underline{\mathbf{H}}^{\mathbf{x}}_{ij}|, \overline{\mathbf{H}}^{\mathbf{x}}_{ij}\right\}$, where $i \neq j$. $\underline{\lambda}_i$ is the lower bound on the curvature of f as estimated by the interval Gerschgorin Theorem. When $\underline{\lambda}_i$ is negative a valid α_i is determined from convexity considerations as $\frac{-\underline{\lambda}_i}{2}$. We see from Table 5 that α_1^1 is bounded by convexity considerations while α_2^3 is bounded by underestimation considerations. The negative of the perturbation function $q(x)$, plotted in Figure 11, in nonconvex and significantly tighter than the perturbation functions depicted in Figure 4.

Table 5. Parameters defining $q_1(x_1)$ and $q_2(x_2)$ for Lennard-Jones potential with negative $\alpha_1^1 < 0$ and $\alpha_2^3 < 0$

k	x_1^k	$\underline{\lambda}_1$	α_1^k	β_1^k	γ_1^k
0	0.00				
1	0.50	1.700	−0.8500	0.69297	0.00000
2	0.75	−4.925	2.4625	0.50234	0.09531
3	1.00	−14.200	7.1000	−1.88828	1.88828
	x_2^k	$\underline{\lambda}_2$	α_2^k	β_2^k	γ_2^k
0	0.00				
1	0.25	−9.000	4.500	1.5000	0.00000
2	0.50	−6.000	3.000	−0.3750	0.46875
3	1.00	3.000	−1.125	−0.5625	0.56250

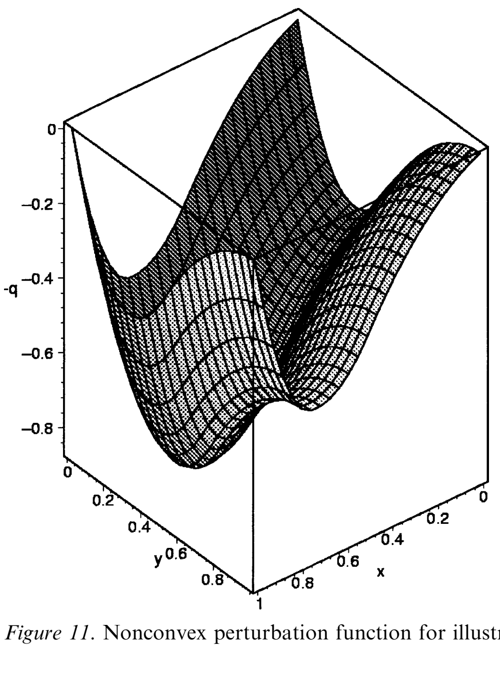

Figure 11. Nonconvex perturbation function for illustration 2.

5.5. DOMAIN SPLITTING

While the aforementioned strategy for determining good underestimators through the use of nonconcave perturbations is useful, the requirement that stationary points be excluded from all convex regions of the perturbation function may be too restrictive to allow the underestimator to be strengthened. The following illustration demonstrates such a case.

Illustration 4: Consider the function $f(x) = \sin(x)$ on the domain $x \in [0, 3\pi]$. The second derivative of this function is $f''(x) = -\sin(x)$. Let the domain be partitioned into 24 equal intervals where the end points are defined such that $x^k = \frac{k\pi}{8}$. A valid underestimation function can be derived by setting

$$\alpha^k = \sin\left(\frac{k\pi}{8}\right), \quad k = 1, \ldots, 4,$$
$$\alpha^k = \sin\left(\frac{(k-1)\pi}{8}\right), \quad k = 5, \ldots, 8,$$
$$\alpha^k = 0, \quad k = 8, \ldots, 16,$$
$$\alpha^k = \sin\left(\frac{k\pi}{8}\right), \quad k = 17, \ldots, 20,$$
$$\alpha^k = \sin\left(\frac{(k-1)\pi}{8}\right), \quad k = 21, \ldots, 24.$$

In the interval $[x^8, x^{16}]$, $f''(x)$ is positive so the α values in these regions may be negative while maintaining the convexity of $\phi(x)$. However, if the stationary point condition (13) is enforced it is found that $|\zeta| \leqslant 10^{-8}$ in this interval and therefore the attainable improvement is negligible. This is because condition (13) is too restrictive, precluding a stationary point from existing in the interval $[x^8, x^{16}]$, whereas the ideal position for a stationary point would be at $\frac{3\pi}{2}$. The underestimator is depicted in Figure 12.

This phenomenon occurs when the convex regions of f lie within the interior of an interval. In the following proposition it is shown that the α's defining a valid convex underestimator may be computed by partitioning the interval of interest, applying Proposition 5.5 to each of the resulting subintervals, then computing the β and γ parameters using the full interval.

PROPOSITION 5.6. *Let $\underline{x} \in \mathbb{R}$ and $\overline{x} \in \mathbb{R}$ define an interval $[\underline{x}, \overline{x}]$. This interval is partitioned into N subintervals defined by x^k, $k = 0, \ldots, N$, where $\underline{x} = x^0 < x^1 < \cdots < x^k < \cdots < x^N = \overline{x}$. Let $q_{ij}(x) : [x^i, x^j] \to \mathbb{R}$ denote a smooth, piecewise quadratic function with the following properties:*

$$q''_{ij}(x) = -2\alpha^k \quad \text{for all}\, x \in [x^{k-1}, x^k]$$

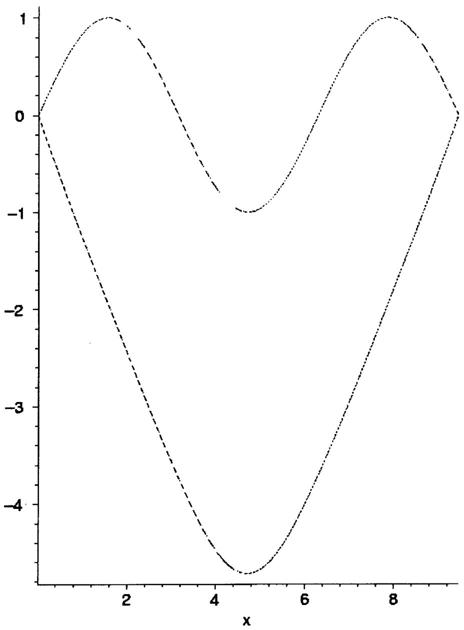

Figure 12. $\sin(x)$ and an underestimator $\sin(x) - q(x)$.

and

$$q_{ij}(x^i) = 0, \qquad q_{ij}(x^j) = 0.$$

If $q_{IJ}(x) \geqslant 0$ *for all* $x \in [x^I, x^J]$ *and* $q_{JK}(x) \geqslant 0$ *for all* $x \in [x^J, x^K]$ then $q_{IK}(x) \geqslant 0$ *for all* $x \in [x^I, x^K]$, *where* $x^0 \leqslant x^I < x^J < x^K \leqslant x^N$.

Proof. First note the following properties of the derivatives of q_{ij} at the end points x^i and x^j,

$$q'_{ij}(x^i) \geqslant 0,$$
$$q'_{ij}(x^j) \leqslant 0.$$

These properties follow from the positivity of q_{ij} on $[x^i, x^j]$ and the end point conditions, $q_{ij}(x^i) = 0$, and $q_{ij}(x^j) = 0$. Now consider the change in the slope between x^i and x^j.

$$q'_{ij}(x^j) - q'_{ij}(x^i) = \int_{x^i}^{x^j} q''_{ij}(x)\,\mathrm{d}x = -\sum_{k=i+1}^{j} 2\alpha^k (x^k - x^{k-1}).$$

Using these expressions with the endpoint properties,

$$q'_{IJ}(x^J) = q'_{IJ}(x^I) - \sum_{k=I+1}^{J} 2\alpha^k (x^k - x^{k-1}) \leqslant 0,$$

$$q'_{JK}(x^J) = q'_{JK}(x^K) + \sum_{k=J+1}^{K} 2\alpha^k (x^k - x^{k-1}) \geqslant 0.$$

The function q_{IK} is smooth, therefore $q'_{IK}(x^J)$ is well defined,

$$q'_{IK}(x^J) = q'_{IK}(x^I) - \sum_{k=I+1}^{J} 2\alpha^k(x^k - x^{k-1})$$

$$= q'_{IK}(x^K) + \sum_{k=J+1}^{K} 2\alpha^k(x^k - x^{k-1}).$$

From this we derive the following inequality:

$$- q'_{IJ}(x^I) + \sum_{k=I+1}^{J} 2\alpha^k(x^k - x^{k-1})$$

$$+ q'_{IK}(x^J) + q'_{JK}(x^K) + \sum_{k=J+1}^{K} 2\alpha^k(x^k - x^{k-1}) - q'_{IK}(x^J) \geqslant 0,$$

which, on cancelling terms, becomes

$$(-q'_{IJ}(x^I) + q'_{IK}(x^I)) + (q'_{JK}(x^K) - q'_{IK}(x^K)) \geqslant 0.$$

Introducing the notation $\Delta^I := q'_{IK}(x^I) - q'_{IJ}(x^I)$ and $\Delta^K := q'_{IK}(x^K) - q'_{JK}(x^K)$

$\Delta^K \leqslant \Delta^I$.

From the endpoint properties of q_{IK},

$$q_{IK}(x^K) - q_{IK}(x^I) = \int_{x^I}^{x^K} q'_{IK}(x)\mathrm{d}x = \int_{x^I}^{x^J} q'_{IJ}(x)$$

$$+ \Delta^I \mathrm{d}x + \int_{x^J}^{x^K} q'_{JK}(x) + \Delta^K \mathrm{d}x = \Delta^I(x^J - x^I) + \Delta^K(x^K - x^J) = 0.$$

Hence, $\Delta^K \leqslant 0$ and $\Delta^I \geqslant 0$. The required result follows: for $x \in [x^I, x^J]$

$$q_{IK}(x) = \int_{x^I}^{x} q'_{IK}(t)\mathrm{d}t = \int_{x^I}^{x} q'_{IJ}(t) + \Delta^I \mathrm{d}t = q_{IJ}(x) + \Delta^I(x - x^I) \geqslant 0$$

as $q_{IJ}(x) \geqslant 0$, $\Delta^I \geqslant 0$ and $(x - x^I) \geqslant 0$; for $x \in [x^J, x^K]$

$$q_{IK}(x) = \int_{x^K}^{x} q'_{IK}(t)\mathrm{d}t = \int_{x^K}^{x} q'_{JK}(t) + \Delta^K \mathrm{d}t = q_{JK}(x) + \Delta^K(x - x^K) \geqslant 0$$

as $q_{JK}(x) \geqslant 0$, $\Delta^K \leqslant 0$ and $(x - x^K) \leqslant 0$.

Illustration 4 continued: This example shows how the underestimation of the function in Illustration 4 can be tightened using Proposition 5.6. As before, the domain is partitioned into 24 equal intervals and the eigenvalue intervals are calculated. As seen in the previous illustration, $f''(x)$ is positive in the interval $[x^8, x^{16}]$ so the α values in these regions may be negative while maintaining the convexity of $\phi(x)$. Instead of computing the underestimator over the interval $[x^0, x^{24}]$ we first calculate the underestimators over each of the intervals $[x^0, x^{12}]$ and $[x^{12}, x^{24}]$ separately. In this way a stationary point may be introduced in the interval $[x^8, x^{16}]$ at x^{12}. The calculations over the two subintervals are carried out as before and only the α values from these calculations are saved (Table 6). Using these α values the β and γ are calculated over the *entire* interval $[x^0, x^{24}]$. From Proposition 5.6 the underestimator derived from this calculation is guaranteed to be a convex underestimator of $f(x)$ (Table 6).

The underestimator is depicted in Figure 13 and the perturbation function q is represented in Figure 14. Notice the nonconcavity of q and the presence of a local minimum at x^{12}.

6. Implementation

Two aspects of the implementation of the α-spline underestimators are discussed in this section, the partitioning of the domain, and the construction of the convex underestimators. The key to the efficient computation of the underestimator lies in the storage and reuse of interval Hessian data. A binary tree is an appropriate data structure for the management of this data. The upper and lower bounds that define the subregion of a partition of the domain are saved at each node of this tree. In addition, estimated ranges of the α's are saved at the leaf nodes. In particular, upper and lower bounds on the α values that pertain to the the region, are saved. The upper bound, $\bar{\alpha}_i^{\mathbf{x}}$, on the α_i required to convexify the nonconvex function $f:(x_1, \ldots, x_n) \to \mathbb{R}$ over a domain $\mathbf{x}$ is defined using the interval Gerschgorin formula,

$$\bar{\alpha}_i^{\mathbf{x}} := -0.5\left(\underline{\mathbf{H}}_{ii}^{\mathbf{x}} - \sum_{j \neq i} \max\left\{|\underline{\mathbf{H}}_{ij}^{\mathbf{x}}|, |\overline{\mathbf{H}}_{ij}^{\mathbf{x}}|\right\}\right).$$

Table 6. sin(x) α values

i	α_i	i	α_i
1	0.19134	13	−0.46193
2	0.35355	14	−0.35355
3	0.46194	15	−0.19134
4	0.50000	16	0.00000
5	0.50000	17	0.19134
6	0.46194	18	0.35355
7	0.35355	19	0.46194
8	0.19134	20	0.50000
9	0.00000	21	0.50000
10	−0.19134	22	0.46194
11	−0.35355	23	0.35355
12	−0.46193	24	0.19134

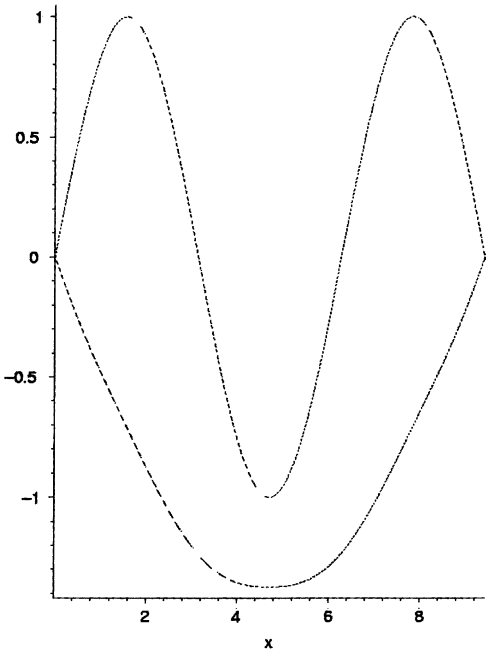

Figure 13. $\sin(x)$ and an underestimator $\sin(x) - q(x)$.

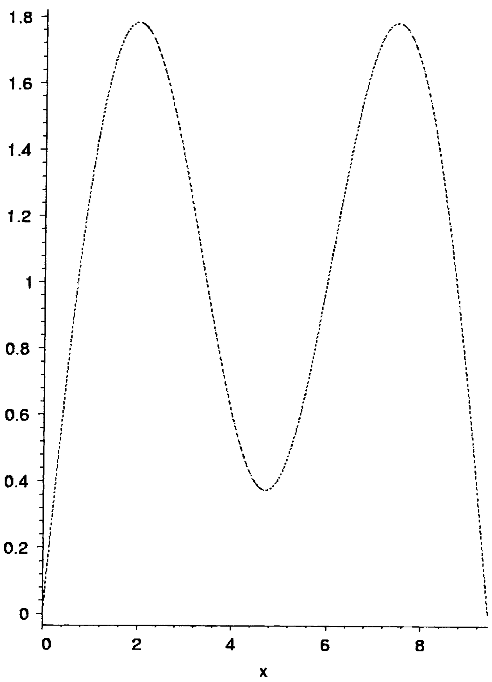

Figure 14. Perturbation function $q(x)$.

This formula differs from that proposed by Adjiman et al. (1998b) in allowing $\overline{\alpha}_i$ to take positive values. In a similar way a lower bound, $\underline{\alpha}_i^{\mathbf{x}}$ on α_i over $\mathbf{x}$ may be defined,

$$\underline{\alpha}_i^{\mathbf{x}} := -0.5\left(\overline{\mathbf{H}}_{ii}^{\mathbf{x}} - \sum_{j\neq i,\ 0\notin|\mathbf{H}_{ij}^{\mathbf{x}}} \min\left\{|\underline{\mathbf{H}}_{ij}^{\mathbf{x}}|, |\overline{\mathbf{H}}_{ij}^{\mathbf{x}}|\right\}\right).$$

In the sequel we will refer to the partitioning of the *problem domain* in the course of a *branch and bound* process as the *branch and bound* partition. The partition that results from the partitioning of a *function domain* for the purposes of constructing an α-spline underestimator of that function will be called the α-spline partition.

6.1. COMPUTATION OF CONVEX UNDERESTIMATORS

Given an α-spline partition the first step in the computation of the underestimator is the extraction of interval and α data from this partition. This is illustrated in Figure 15(a) and (b) which represent an α-spline partition. Figure 15(a) demonstrates the extraction of x_1^k and $\overline{\alpha}_1^k$ data from this partition. To guarantee the convexity of the underestimator the *largest* $\overline{\alpha}_i^k$ over any subinterval $[x_1^{k-l}, x_1^k]$ is required. The shaded regions in Figure 15(a) show those regions of the partition that contribute to the definition of $q_1(x)$. Similarly Figure 15(b) shows the data defining $q_2(x)$. A shaded region in the partition that defines $\overline{\alpha}_i^k$ is denoted $\mathbf{x}^{i,k}$.

In the second step the domain is split into α-adjustment subintervals as discussed in Section 5.5. This is illustrated in Figure 16. In this figure five subregions have negative $\overline{\alpha}$'s. Consecutive intervals with negative $\overline{\alpha}$'s that are flanked by regions with positive $\overline{\alpha}$'s are split so that any consecutive set of such intervals lies at an end of an α-adjustment subinterval. The two α-adjustment subintervals resulting from this operation are indication by the

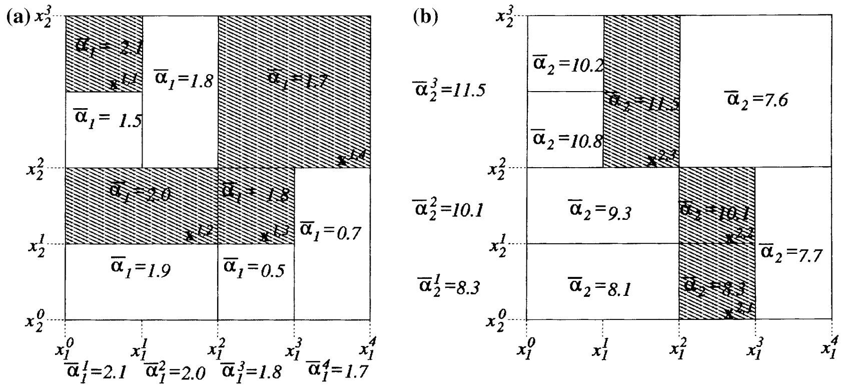

Figure 15. Extraction of α values for α-spline calculation.

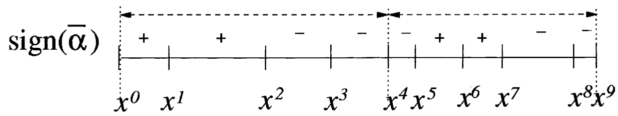

Figure 16. Domain splitting for α-adjustment.

dashed intervals in Figure 16. The α's associated with intervals with negative $\overline{\alpha}$'s are initialized to zero then adjusted, as in Section 5 to values between 0 and $\overline{\alpha}$.

Finally, the β and γ parameters are computed using Equations 7–9.

6.2. DOMAIN PARTITIONING

The manner and extent to which the domain is (α-spline) partitioned influences both the tightness of the underestimators as well as the cost of calculating them. Here a relatively simple α-spline partitioning approach is proposed wherein the domain is partitioned into a grid at the root node of the branch and bound tree and refined as the branch and bound tree expands. The initial grid for the α-spline underestimator of a function $f(x_1, \ldots, x_n)$ is constructed through the recursive bisection of the intervals of the variables. A parameter N_{init} defines the number of initial bisections to be used in the construction of this grid into $2^{N_{\text{init}}}$ regions. To keep the size of the α-spline partition to a manageable size we define a parameter $N_{\max}$. At any iteration of the branch and bound algorithm further partitioning of the α-spline partition occurs only if the number of regions in this partition that intersect with the current *branch and bound* region is less than $N_{\max}$. In Figure 17(a) the initial partition is defined using the parameter $N_{\text{init}} = 5$. Figure 17(b) shows the the branch and bound and the α-spline partition on the sixth iteration where the parameter $N_{\max} = 2$. The regions of the *branch and bound* partition labelled A, B and C each include eight regions of the α-*spline* partition. No refinement of the α-*spline* partition is to be done in these regions as 8 exceeds $N_{\max}$. Similarly D cannot be refined as this region contains four α-*spline* regions. The α-*spline* partition will be refined in the E and F regions when these *branch and bound*

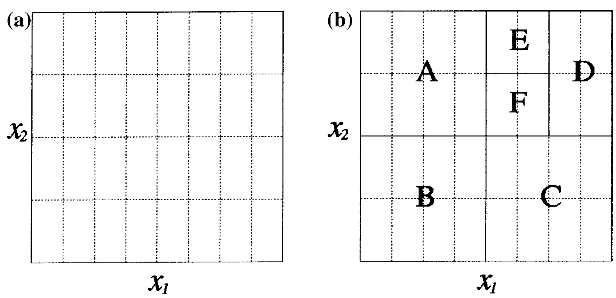

Figure 17. Branch-and-bound and α-spline underestimator partitioning.

nodes are processed. The refinement of an α-spline partition at nodes of the branch and bound tree that are not root nodes occurs as follows. First, the region $\mathbf{x}'$ of the α-spline partition that has the largest influence on the strength of the underestimation is selected based on the criterion,

$$\max_k \max_i (x_i^k - x_i^{k-1})(\overline{\alpha}_i^k - \underline{\alpha}_i^k).$$

The index of the variable along which the chosen region is bisected is then chosen as

$$\arg\max_j \left(\overline{\mathbf{H}}_{ij}^{\mathbf{x}'} - \underline{\mathbf{H}}_{ij}^{\mathbf{x}'}\right)(\overline{x}_j - \underline{x}_j).$$

7. Computational Experiments

A set of computational experiments were carried out to assess whether the gains in the convergence rate of a branch and bound algorithm can offset the computational cost of calculating the α-spline functions. The αBB algorithm as implemented in C by Adjiman et al. (1998a) was augmented with an implementation of the α-spline convex underestimators. Comparisons between the α-spline underestimator defined using a range of N_{init} and $N_{\max}$ parameters demonstrate the effect of the α-spline partitioning strategy.

7.1. SIX-HUMP CAMELBACK FUNCTION

The following function is known as the Six-Hump Camelback function (Dixon and Szegö, 1975),

$$f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4.$$

Two problems based on this function were used as a basis of comparison between solution strategies.

Six-Hump Camelback function: A bound constrained minimization problem with six local solutions was formulated with the objective function,

$$\min_{x \in [-2.0, 2.0]^2} f(x_1, x_2).$$

The global solution to this problem is $(x_1^*, x_2^*) = (0.08984, -0.71266)$, where the objective function is $f(x_1^*, x_2^*) = -1.03163$.

In these computational tests the lower bounding problem was formulated as,

$$\min_{x \in \mathbf{x}} \underline{f}(x_1, x_2),$$

where $\mathbf{x}$ is the domain. This problem was solved using the αBB algorithm without acceleration techniques such as domain reduction. Convergence was based on the criterion $(\text{UB} - \text{LB}) \leqslant 1 \times 10^{-6}$ where UB denotes the best known upper bound on the solution and LB a rigorous lower bound on the global solution. The results of seven runs are summarized in Table 7. N_{init} defines the initial grid structure as discussed in Section 6.2. Subsequent refinement is controlled by the parameter $N_{\max}$. The lower bound found at the root node is denoted LB^0 in this table. The number of iterations and the CPU time on an HP J2240 are labelled "iters" and "CPU", respectively.

The first line of this table refers to the performance of the classical αBB approach using the scaled Gerschgorin method for the calculation of α's. All runs using the α-spline underestimator performed better than the classical αBB. The number of iterations for convergence decreases with increasing grid refinement, as expected. The CPU time shows a similar trend, except for $N_{\text{init}} = 2$.

Triple Six-Hump Camelback function: A more complex bound constrained minimization problem was formulated based on a nonseparable objective function which is the sum of three Six-Hump Camelback functions,

$$\min_{x \in [-2.0, 2.0]^4} f(x_1, x_2) + f(x_2, x_3) + f(x_3, x_4).$$

The lower bounding problem was formulated as follows:

$$\begin{aligned} &\min_{x \in \mathbf{x}, w \in \mathbf{w}} \quad w_1 + w_2 + w_3 \\ &\text{subject to} \\ &\underline{f}(x_1, x_2) \leqslant w_1, \\ &\underline{f}(x_2, x_3) \leqslant w_2, \\ &\underline{f}(x_3, x_4) \leqslant w_3. \end{aligned}$$

The αBB approach was applied to this problem, with branching on x variables only, and bound updates on the w variables only. Table 8 summarizes the results of seven runs. As before the α-spline based underestimation scheme performed better than the classical αBB in all cases. Note that the improvement in the computational performance is

Table 7. Computational results for Six-Hump Camelback function

N_{init}	$N_{\max}$	LB^0	iters	CPU (s)
0	0	-3.753×10^2	61	0.57
1	256	-2.056×10^2	38	0.42
2	256	-1.508×10^2	38	0.50
3	256	-8.720×10^1	38	0.38
4	256	-7.030×10^1	36	0.37
5	256	-4.130×10^1	33	0.37
6	256	-3.602×10^1	30	0.35

Table 8. Computational results for triple Six-Hump Camelback function

N_{init}	N_{max}	LB^0	iters	CPU (s)
0	0	-11.256×10^2	4971	64.98
1	16	-6.168×10^2	1111	20.27
1	256	-6.168×10^2	665	15.34
2	16	-4.519×10^2	1111	20.21
2	256	-4.519×10^2	663	15.38
4	16	-2.408×10^2	1111	20.13
4	256	-2.095×10^2	663	15.32

greater in this problem simply because there are more variables that participate in α-underestimated nonconvex functions in this problem. From this table we observe that in this problem the structure of the initial grid appears to be less influential than the refinement of this grid.

7.2. SHUBERT FUNCTION

The problems in this section are based on the Shubert function,

$$f(x) := \sum_{i=1}^{5} i\cos((1+i)x+i),$$

a multimodal test function for testing nonlinear programming algorithms. The convergence tolerance $\frac{(UB-LB)}{|LB|} \leqslant 0.001$ was used for the problems based on the Shubert function.

Shubert function: The following bound constrained minimization problem entails the minimization of the Shubert function,

$$\min_{x\in[-10,10]} f(x).$$

Table 9 shows trends similar to those of Table 8. Refinement of the α-spline partition generally lead to improved performance. In the final run (line 7) the CPU time increased slightly relative to that of the previous run even though the number of iterations required for convergence decreased. There was also a small increase in CPU time between the runs in lines 2 and 7.

Table 9. Computational results for Shubert function

N_{init}	N_{max}	iters	CPU (s)
0	0	2237	586.82
2	16	489	161.33
2	64	297	122.76
2	256	217	119.66
4	16	489	160.28
4	64	296	120.20
4	256	217	120.97

Double Shubert function: The Shubert function was used to construct a more complex "double Shubert" function in the following minization problem:

$$\min_{x\in[-10,10]^3} f(x_1)f(x_2)+f(x_2)f(x_3).$$

The lower bounding problem was formulated in two ways which will be referred to as "**A**" and "**B**".
In formulation **A** the function

$$g(x_1,x_2)=f(x_1)f(x_2)$$

is treated as a general C^2 continuous function and the lower bounding problem is formulated applying α underestimators to bivariate functions. The following lower bounding formulation results:

$$\min_{x\in[-10,10]^3} \underline{g}(x_1,x_2)+\underline{g}(x_2,x_3). \tag{A}$$

The lower bounding formulation **B** is as follows:

$$
\begin{aligned}
&\min_{x\in[-10,10]^3 w\in\mathbb{R}^5} w_4+w_5\\
&\text{subject to}\\
&\underline{f}(x_1)\leqslant w_1,\\
&\underline{f}(x_2)\leqslant w_2,\\
&\underline{f}(x_3)\leqslant w_3,\\
&\underline{w_2}w_1+\underline{w_1}w_2+\underline{w_1w_2}\leqslant w_4,\\
&\overline{w_2}w_1+\overline{w_1}w_2+\overline{w_2w_1}\leqslant w_4,\\
&\underline{w_2}w_3+\underline{w_3}w_2+\underline{w_2w_3}\leqslant w_5,\\
&\overline{w_2}w_3+\overline{w_3}w_2+\overline{w_2w_3}\leqslant w_5.
\end{aligned} \tag{B}
$$

In this formulation the objective function is underestimated through the introduction of auxiliary variables $w_1,\ldots,w_5$, the use of convex envelopes for the underestimation of bilinear terms (McCormick, 1976), and the use of α-spline underestimators for the underestimation of the *univariate* Shubert function.

Computational results for both formulations are tabulated in Table 10. The α-spline underestimation performed far better than the classical αBB for both formulations. In formulation **A** the classical αBB took 341% of the iterations required by the α-spline method and in formulation **B** this percentage increased to 51,252%. These results can be attributed primarily to the quality of the α-spline underestimator being better for *univariate* functions that for *bivariate* ones.

Table 10. Double Shubert function computational results

	N_{init}	N_{max}	iters	CPU (s)
A	0	0	250952	34169
	4	256	73427	6303
B	0	0	51150	62021
	4	256	998	1672

The progress of the upper and lower bounds is shown in Figure 18(a) and (b) for formulations **A** and **B**. In both of these figures we note a bumpy convergence of the classical αBB lower bound and a much smoother convergence of the α-spline lower bound. Relatively small regions of the problem domain in which the objective function is very *concave* influence the classical αBB underestimators to a larger degree than they influence the α-spline underestimators resulting in this convergence behaviour.

8. Conclusion

The refinement of the αBB convex underestimator, proposed in this paper, can be significantly tighter than the classical αBB underestimator. In some cases the underestimator closely approximates the convex envelope. The perturbation function, a smooth, piecewise quadratic, function with varying curvature, may be nonconvex, yet is guaranteed to form a convex underestimator when subtracted from the function being underestimated. The main computational effort in the calculation of the parameters of the α-spline underestimator lies in the evaluation of the interval Hessian matrix in a potentially large number of subregions of the function domain. This effort can be offset by storing the interval Hessian data that are generated at the nodes in the branch and bound tree and reusing this information in other nodes of the tree. Computational results show

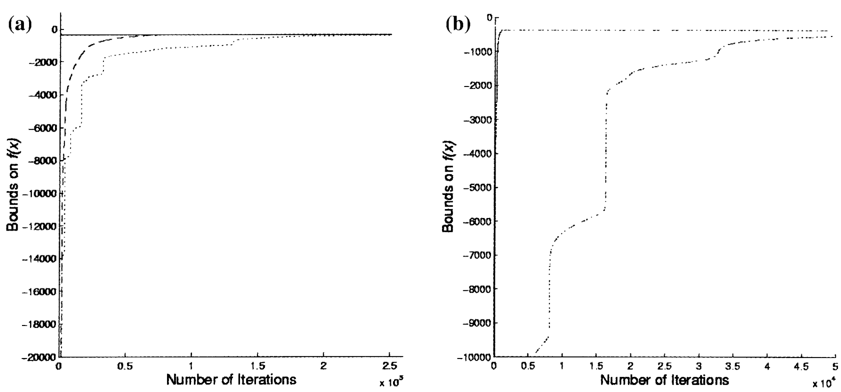

Figure 18. Double Shubert function computational results.

that the proposed underestimator is indeed more effective then the classical approach.

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