Journal of Global Optimization (2005) 33: 83–107
DOI 10.1007/s10898-004-6100-2

Proof of Convergence for a Global Optimization Algorithm for Problems with Ordinary Differential Equations

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(Received 23 December 2003; accepted 10 November 2004)

Abstract. A deterministic spatial branch and bound global optimization algorithm for problems with ordinary differential equations in the constraints has been developed by Papamichail and Adjiman [A rigorous global optimization algorithm for problems with ordinary differential equations. J. Glob. Optim. **24**, 1–33]. In this work, it is shown that the algorithm is guaranteed to converge to the global solution. The proof is based on showing that the selection operation is bound improving and that the bounding operation is consistent. In particular, it is shown that the convex relaxation techniques used in the algorithm for the treatment of the dynamic information ensure bound improvement and consistency are achieved.

Key words: Deterministic global optimization, ordinary differential equations, proof of convergence

1. Introduction

Dynamic optimization problems are of great practical importance and a number of methods can be applied for their solution (Sargent, 2000). One class of approaches uses variable discretization in order to transform the problem to a finite dimensional NLP. In complete discretization (known as the simultaneous approach) both the state variables and the controls are discretized (Tsang et al., 1975; Oh and Luus, 1997; Biegler, 1984). The solution is carried out in the full space of variables. However, this method results in an NLP problem with a large number of variables and nonlinear equality constraints. In control parameterization (known as the sequential approach) only the controls are discretized (Pollard and Sargent, 1970; Sargent and Sullivan, 1978; Goh and Teo, 1988; Vassiliadis et al., 1994). The problem is solved using an NLP strategy. The dynamic system is decoupled from the optimization stage and is integrated using well-established techniques in order to evaluate the objective function and the constraints. However, due to the nonconvexity of these formulations, only local solutions can be identified by most of the established gradient-based NLP solvers.

Recently, deterministic global optimization algorithms have been applied for the solution of dynamic optimization problems. Smith and Pantelides (1996) applied their symbolic manipulation and spatial branch and bound (BB) algorithm. Esposito and Floudas (2000a,b) used the αBB method (Maranas and Floudas, 1994; Androulakis et al., 1995; Adjiman and Floudas, 1996; Adjiman et al., 1998a,b). Singer and Barton (2002) presented a theory that can be utilized in a BB algorithm for the global solution of linear dynamic embedded problems. Barton and Lee (2003) have extended this approach to linear hybrid systems.

The authors (Papamichail and Adjiman, 2002) have proposed a deterministic spatial BB global optimization algorithm for problems with ordinary differential equations (ODEs) in the constraints. Bilinear terms, univariate concave terms and general twice continuously differentiable terms can be tackled. A rigorous approach has been developed for the convex relaxation of the dynamic information. The concept of differential inequalities has been used to construct bounds on the space of solutions of parameter dependent ODEs as well as on their second-order sensitivities. Recently, an alternative convex relaxation based on the construction of linear dynamic systems has been proposed (Papamichail and Adjiman, 2004) and incorporated within the algorithm. This algorithm was applied successfully to several case studies, using different combinations of the convex relaxations. The proof of convergence for this algorithm is discussed in this paper. In particular, it is shown that the convex relaxation proposed by Papamichail and Adjiman (2002) has the necessary properties to ensure convergence of the algorithm. The use of the convex relaxation based on linear dynamic systems is not necessary to prove convergence and is therefore not considered here.

The statement of the dynamic optimization problem is given in Section 2. The global optimization algorithm is presented in Section 3. These first two sections provide the key concepts and notation needed for the proof. Bound improvement is then discussed in Section 4 where the properties of the new convex relaxation procedure are exploited. The consistency of the bounding operation is presented in Section 5. Based on these two properties, the proof of convergence follows.

2. Problem statement

DEFINITION 2.1. Let $\mathcal{I}=[t_0, t_{NS}] \subset \Re$, $\mathcal{I}_0 = (t_0, t_{NS}]$, $x = (x_1, x_2, \ldots, x_n)^T$ and $x_{k^-} = (x_1, x_2, \ldots, x_{k-1}, x_{k+1}, \ldots, x_n)^T$. The following notation is used: $f(t, x) = f(t, x_k, x_{k^-})$.

The formulation of the dynamic optimization problem studied is given by:

$$
\begin{aligned}
&\min_{p} J(x(t_i, p), p\,;\ i=0,1,\ldots,NS)\\
&\text{s.t.}\\
&\qquad \dot{x} = f(t, x, p)\ \forall t \in \mathcal{I}\\
&\qquad x(t_0) = x_0(p)\\
&\qquad g_i(x(t_i, p), p) \leqslant 0\,,\ i=0,1,\ldots,NS\\
&\qquad p^L \leqslant p \leqslant p^U
\end{aligned}
\tag{1}
$$

where $t_i \in \mathcal{I}$, $x \in \Re^n$ are the state variables, $\dot{x} \in \Re^n$ are their derivatives with respect to t, and $p \in \Re^r$ are the parameters. The functions J, f, x_0 and g_i, $i=0,1,\ldots,NS$, are such that $J : \Re^{n\cdot(NS+1)} \times \Re^r \mapsto \Re$, $f : \mathcal{I} \times \Re^n \times \Re^r \mapsto \Re^n$, $x_0 : \Re^r \mapsto \Re^n$ and $g_i : \Re^n \times \Re^r \mapsto \Re^{s_i}$.

Systems with controls that depend on t can be transformed to this form using control parameterization (Vassiliadis et al., 1994).

Remark 2.1. The following assumptions are made:

- $J(x(t_i, p), p;\ i=0,1,\ldots,NS)$ is twice continuously differentiable with respect to $x(t_i, p)$, $i=0,1,\ldots,NS$ and p on $\Re^{n\cdot(NS+1)} \times \Re^r$.
- Each element of $g_i(x(t_i, p), p)$ is twice continuously differentiable with respect to $x(t_i, p)$ and p, $i=0,1,\ldots,NS$ on $\Re^n \times \Re^r$.
- Each element of $f(t, x, p)$ is continuous with respect to t and is twice continuously differentiable with respect to the states x and the parameters p on $\mathcal{I} \times \Re^n \times \Re^r$.
- Each element of $x_0(p)$ is twice continuously differentiable with respect to the parameters p on $\Re^r$.
- $f(t, x, p)$ satisfies a uniqueness condition (see 12.IVa of Walter, 1970) on $\mathcal{I} \times \Re^n \times \Re^r$.

The sequential approach (Vassiliadis et al., 1994) is used for the local solution of this dynamic optimization problem. Given values for the parameters p, the ODE system, included in the constraints of problem (1), can be integrated from t_0 to t_{NS} using a standard numerical technique. After reaching t_{NS}, the objective function and the constraints can be evaluated. The evaluation of their gradients with respect to p can be done using the parameter sensitivities. These are given from the solution of the sensitivity equations:

$$\dot{x}_p(t, p) = \frac{\partial f}{\partial x} x_p(t, p) + \frac{\partial f}{\partial p} \qquad \forall t \in \mathcal{I},$$

where:

$$x_p(t, p) = \frac{\partial x}{\partial p}$$

and

$$\dot{x}_p(t,p)=\frac{\partial}{\partial t}\left(\frac{\partial x}{\partial p}\right).$$

The initial condition for the sensitivity equations is given by:

$$x_p(t_0,p)=\frac{\partial x_0}{\partial p}.$$

Remark 2.2. The solution $x(t_i,p)$ of the ODE in problem (1) with the initial condition specified is twice continuously differentiable with respect to the parameters p on $\Re^r$ (Papamichail and Adjiman, 2002).

3. Global optimization algorithm

The deterministic spatial BB global optimization algorithm for problems with ODEs in the constraints that was developed by Papamichail and Adjiman (2002) is presented briefly in this section. The convex relaxed problem is first formulated. Each step of the algorithm is then presented.

3.1. FORMULATION OF THE CONVEX RELAXATION

A reformulation of the NLP problem (1) is given by:

$$\begin{aligned}
&\min_{\hat{x},p} J(\hat{x},p)\\
&\text{s.t.}\\
&\quad g_i(\hat{x}_i,p)\leqslant 0, \quad i=0,1,\ldots,NS\\
&\quad \hat{x}_i=x(t_i,p), \quad i=0,1,\ldots,NS\\
&\quad p\in[p^L,p^U]
\end{aligned} \tag{2}$$

where the values of $x(t_i,p)$, $i=0,1,\ldots,NS$ are obtained by solving the ODE system:

$$\dot{x}(t,p)=f(t,x(t,p),p) \quad \forall t\in\mathcal{I} \tag{3}$$

$$x(t_0,p)=x_0(p). \tag{4}$$

3.1.1. *Bounds on* $\hat{x}_i$

The following remark can be used to construct bounds for the solutions of ODE system (3)–(4).

Remark 3.1. If f is continuous and satisfies a uniqueness condition on $\mathcal{I}_0\times\Re^n\times[p^L,p^U]$ then the solution of the following ODE system satisfies Theorem 3.3 in Papamichail and Adjiman (2002):

$$\begin{aligned}
&\dot{\underline{x}}_k(t) = \inf f_k(t, \underline{x}_k(t), [\underline{x}_{k^-}(t), \overline{x}_{k^-}(t)], [p^L, p^U]) \\
&\dot{\overline{x}}_k(t) = \sup f_k(t, \overline{x}_k(t), [\underline{x}_{k^-}(t), \overline{x}_{k^-}(t)], [p^L, p^U]) \\
&\qquad \forall t \in \mathcal{I} \quad \text{and} \quad k = 1, 2, \ldots, n
\end{aligned} \tag{5}$$

$$\begin{aligned}
&\underline{x}(t_0) = \inf x_0([p^L, p^U]) \\
&\overline{x}(t_0) = \sup x_0([p^L, p^U])
\end{aligned} \tag{6}$$

which means that $\underline{x}(t)$ is a subfunction and $\overline{x}(t)$ is a superfunction for the set of solutions of the ODE that appears in the constraints of the NLP problem (1), i.e.,

$$\underline{x}(t) \leqslant x(t, p) \leqslant \overline{x}(t) \quad \forall p \in [p^L, p^U] \quad \forall t \in \mathcal{I},$$

where the inequalities are understood component-wise. Natural interval extensions (Moore, 1966) are used as inclusion functions and directed outward rounding is applied to the calculations in the system (5)–(6).

These bounds are also valid for the variable vectors $\hat{x}_i$ that have been introduced in the reformulated NLP problem:

$$\underline{x}(t_i) \leqslant \hat{x}_i \leqslant \overline{x}(t_i), \quad i = 0, 1, \ldots, NS. \tag{7}$$

3.1.2. *Convex relaxation of J and g_i*

Any function $q(z)$, which can be decomposed into a sum of convex, bilinear, univariate concave and general nonconvex twice continuously differentiable terms, can be written as

$$q(z) = f_{CT}(z) + \sum_{i=1}^{bt} b_i z_{B_i,1} z_{B_i,2} + \sum_{i=1}^{ut} f_{UT,i}(z_{UT,i}) + \sum_{i=1}^{nt} f_{NT,i}(z), \tag{8}$$

where $f_{CT}(z)$ is a convex term, bt is the number of bilinear terms, $z_{B_i,1}$ and $z_{B_i,2}$ are the two variables in the ith bilinear term with coefficient b_i, ut is the number of univariate concave terms, $f_{UT,i}(z_{UT,i})$ is the ith univariate concave term, $z_{UT,i}$ is the variable in the ith univariate concave term, nt is the number of general nonconvex terms and $f_{NT,i}(z)$ is the ith general nonconvex term.

It is assumed that the functions J and g_{ij}, $i = 0, 1, \ldots, NS$, $j = 1, 2, \ldots, s_i$ are functions such as $q(z)$. A convex relaxation for $q(z)$ can be derived by constructing a convex relaxation for each term. Convex terms do not require any transformation. Bilinear terms, univariate concave terms and general nonconvex twice continuously differentiable terms are underestimated using well-known techniques.

3.1.2.1. *Underestimating bilinear terms.* The convex envelope for the bilinear term $z_1 z_2$ over the domain $[z_1^L, z_1^U] \times [z_2^L, z_2^U]$ (McCormick, 1976; Al-Khayyal and Falk, 1983) is given by:

$$\max(z_1^L z_2 + z_2^L z_1 - z_1^L z_2^L, z_1^U z_2 + z_2^U z_1 - z_1^U z_2^U).$$

Each bilinear term is replaced by a new variable w defined by $w = z_1 z_2$. In the relaxed problem, this equation has to be replaced by a convex underestimator and a concave overestimator as follows:

$$\begin{aligned} w &\geqslant z_1^L z_2 + z_2^L z_1 - z_1^L z_2^L \\ w &\geqslant z_1^U z_2 + z_2^U z_1 - z_1^U z_2^U \\ w &\leqslant z_1^L z_2 + z_2^U z_1 - z_1^L z_2^U \\ w &\leqslant z_1^U z_2 + z_2^L z_1 - z_1^U z_2^L. \end{aligned} \tag{9}$$

3.1.2.2. *Underestimating univariate concave terms.* For a univariate concave function $f_{UT}(z)$, the convex envelope over the domain $[z^L, z^U]$ is simply given by the linear function of z:

$$f_{UT}(z^L) + \frac{f_{UT}(z^U) - f_{UT}(z^L)}{z^U - z^L}(z - z^L).$$

3.1.2.3. *Underestimating general twice continuously differentiable terms.* For a general twice continuously differentiable function $f_{NT}(z)$ the α-based underestimator (Maranas and Floudas, 1994; Androulakis et al., 1995) can be used over the domain $[z^L, z^U] \subset \Re^m$:

$$f_{NT}(z) + \sum_{i=1}^{m} \alpha_i (z_i^L - z_i)(z_i^U - z_i),$$

where the values for the non-negative α_i parameters are calculated using the scaled Gerschgorin method proposed by Adjiman et al. (1998b). This method requires the use of a symmetric interval matrix $[H_{f_{NT}}] = ([\underline{h}_{ij}, \overline{h}_{ij}])$ such that $[H_{f_{NT}}] \ni H_{f_{NT}}(z) = \nabla^2 f_{NT}(z)$, $\forall z \in [z^L, z^U]$. For any vector $d = (d_1, d_2, \ldots, d_n)^T$ with $d_i > 0, \forall i = 1, 2, \ldots, n$, α_i can be calculated by the following formula:

$$\alpha_i = \max\left\{0, -\frac{1}{2}\left(\underline{h}_{ii} - \sum_{j\neq i} |h|_{ij}\frac{d_j}{d_i}\right)\right\}, \tag{10}$$

where $|h|_{ij} = \max\{|\underline{h}_{ij}|, |\overline{h}_{ij}|\}$. Constant values for the vector d are used in the present algorithm. The interval matrix $[H_{f_{NT}}]$ is calculated by applying natural interval extensions to the analytical expression for each second-order derivative of f_{NT} and is given by $[H_{f_{NT}}] = H_{f_{NT}}([z^L, z^U])$. These values for the α_i parameters guarantee the convexity of the underestimator.

3.1.2.4. *Overall convex underestimator.* An overall convex underestimator of the function introduced by equation (8), $q(z)$, over the domain $[z^L, z^U] \subset \Re^m$ is given by:

$$\begin{aligned}\breve{q}(z, w) = {} & f_{CT}(z) + \sum_{i=1}^{bt} b_i w_i \\ & + \sum_{i=1}^{ut}\left(f_{UT,i}(z^L_{UT,i}) + \frac{f_{UT,i}(z^U_{UT,i}) - f_{UT,i}(z^L_{UT,i})}{z^U_{UT,i} - z^L_{UT,i}}(z_{UT,i} - z^L_{UT,i})\right) \\ & + \sum_{i=1}^{nt}\left(f_{NT,i}(z) + \sum_{j=1}^{m}\alpha_{ij}(z^L_j - z_j)(z^U_j - z_j)\right).\end{aligned}$$

The constraints (9) must also be satisfied for each variable w_i.

3.1.3. *Convex relaxation of the set of equality constraints*

The set of equalities can be written as two sets of inequalities:

$$\begin{aligned}\hat{x}_i - x(t_i, p) \leqslant 0, \quad i = 0, 1, \ldots, NS \\ x(t_i, p) - \hat{x}_i \leqslant 0, \quad i = 0, 1, \ldots, NS.\end{aligned}$$

Their relaxation is given by:

$$\hat{x}_i + \breve{x}^-(t_i, p) \leqslant 0, \quad i = 0, 1, \ldots, NS \tag{11}$$

$$\breve{x}(t_i, p) - \hat{x}_i \leqslant 0, \quad i = 0, 1, \ldots, NS, \tag{12}$$

where the $\breve{}$ superscript denotes the convex underestimator of the specified function and $x^-(t_i, p) = -x(t_i, p)$. The function $\breve{x}(t_i, p)$ is a convex underestimator of $x(t_i, p)$ and the function $-\breve{x}^-(t_i, p)$ is a concave overestimator of $x(t_i, p)$. Two strategies have been developed by Papamichail and Adjiman (2002) to derive these over and underestimators.

3.1.3.1. *Constant bounds.* The constant bounds given by inequalities (7) are valid convex underestimators and concave overestimators for $x(t_i, p)$. This means that inequalities (11) and (12) can be replaced by inequalities (7). These bounds do not depend on the parameters p themselves, but do depend on the bounds on p.

3.1.3.2. *α-based bounds.* Based on Remark 2.2, $x(t_i, p)$ is a twice continuously differentiable function of the parameters p on $\Re^r$. This means that the α-based underestimators can be used for the convex underestimation of $x(t_i, p)$ and $x^-(t_i, p)$ over the domain $[p^L, p^U] \subset \Re^r$ (Esposito and Floudas, 2000a,b):

$$\breve{x}_k(t_i, p) = x_k(t_i, p) + \sum_{j=1}^{r} \alpha^+_{kij}(p^L_j - p_j)(p^U_j - p_j)$$
$$i = 0, 1, \ldots, NS,\ k = 1, 2, \ldots, n$$
$$\breve{x}^-_k(t_i, p) = x^-_k(t_i, p) + \sum_{j=1}^{r} \alpha^-_{kij}(p^L_j - p_j)(p^U_j - p_j)$$
$$i = 0, 1, \ldots, NS,\ k = 1, 2, \ldots, n$$

Papamichail and Adjiman (2002) proposed the following procedure for the calculation of the α^+_{kij} and α^-_{kij} parameters. The scaled Gerschgorin method can be utilized again. Constant values for the vector d are used. Based on Remark 3.1 bounds are constructed for the ODE system that is generated when the first and the second-order sensitivity equations are coupled with the original ODE system (3)–(4). These bounds on the second-order derivatives can then be used to construct each element of the interval Hessian matrices $[H_{x_k(t_i)}] \ni H_{x_k(t_i)}(p) = \nabla^2 x_k(t_i, p),\ \forall p \in [p^L, p^U]$ and $[H_{x^-_k(t_i)}] = -[H_{x_k(t_i)}]$.

3.1.4. *Convex relaxation of the NLP*

After underestimating the objective function and overestimating the feasible region, the convex relaxation of the NLP problem (2) is given by:

$$\begin{aligned}
&\min_{\hat{x}, p, w}\ \breve{J}(\hat{x}, p, w) \\
&\text{s.t.} \\
&\quad \breve{g}_i(\hat{x}_i, p, w) \leqslant 0,\ i = 0, 1, \ldots, NS \\
&\quad \underline{x}(t_i) \leqslant \hat{x}_i \leqslant \overline{x}(t_i),\ i = 0, 1, \ldots, NS \\
&\quad \breve{\mathcal{C}}(\hat{x}, p, w) \leqslant 0 \\
&\quad p \in [p^L, p^U]
\end{aligned} \tag{13}$$

where the ˇ superscript denotes the convex underestimator of the specified function, $\mathcal{C}$ denotes the set of additional constraints arising from the convex relaxation of bilinear terms and w denotes the vector of new variables introduced by this relaxation. If the α-based method is also used for the convex relaxation of the set of equality constraints then the following constraints can be added to the above formulation:

$$\begin{aligned} \hat{x}_i + \check{x}^-(t_i, p) \leqslant 0, \quad i = 0, 1, \ldots, NS \\ \check{x}(t_i, p) - \hat{x}_i \leqslant 0, \quad i = 0, 1, \ldots, NS. \end{aligned} \tag{14}$$

3.2. SPATIAL BB ALGORITHM

After constructing the convex relaxation of the original NLP problem, a spatial BB algorithm, which follows the one by Horst and Tuy (1996), can be used in order to obtain the global minimum within an optimality margin. This algorithm is described in the present subsection. Some steps are then analyzed further.

3.2.1. *Structure of BB algorithm*

Given a relative optimality margin, ϵ_r, and a maximum number of iterations, $MaxIter$:

Step 1: Initialization

Set the upper bound on the objective function: $J^u := +\infty$.
Initialize the iteration counter: $Iter := 0$.
Initialize a list of subregions $\mathcal{L}$ to an empty list: $\mathcal{L} := \emptyset$.
Initialize a region $\mathcal{R}$ to the region covering the full domain of variables p: $\mathcal{R} := [p^L, p^U]$.

Step 2: Upper bound

Solve the original NLP problem with bounds on p given by $\mathcal{R}$.
If a feasible solution $p_{\mathcal{R}}$ is obtained with objective function $J^u_{\mathcal{R}}$, then set the best feasible solution $p^* := p_{\mathcal{R}}$ and $J^u := J^u_{\mathcal{R}}$.

Step 3: Lower bound

Obtain bounds on the differential variables.
If the α-based relaxation is additionally used for the overestimation of the equality constraints then obtain bounds on the second-order sensitivities.
Form the relaxed problem for $\mathcal{R}$ and solve it.
If a feasible solution $p^*_{\mathcal{R}}$ is obtained for $\mathcal{R}$ with objective function $J^\ell_{\mathcal{R}}$, then add $\mathcal{R}$ to the list $\mathcal{L}$ together with $J^\ell_{\mathcal{R}}$ and $p^*_{\mathcal{R}}$.

Step 4: Subregion selection

If the list is empty, then the problem is infeasible. Terminate.
Otherwise set the region $\mathcal{R}$ to the region from the list $\mathcal{L}$ with the lowest lower bound: $\mathcal{R} := \arg\min_{\mathcal{L}_i \in \mathcal{L}} J^{\ell}_{\mathcal{L}_i}$.
Remove $\mathcal{R}$ from the list $\mathcal{L}$.

Step 5: Checking for convergence

If $\frac{J^u - J^{\ell}_{\mathcal{R}}}{|J^{\ell}_{\mathcal{R}}|} \leqslant \epsilon_r$, then terminate. The solution is p^* with an objective function J^u.
If $Iter = MaxIter$, then terminate and report $\frac{J^u - J^{\ell}_{\mathcal{R}}}{|J^{\ell}_{\mathcal{R}}|}$.
Otherwise increase the iteration counter by one: $Iter := Iter + 1$.

Step 6: Branching within $\mathcal{R}$

Apply a branching rule on subregion $\mathcal{R}$ to choose a variable on which to branch and generate two new subregions, $\mathcal{R}_1, \mathcal{R}_2$ which are a partition of $\mathcal{R}$.

Step 7: Upper bound for each region

For $i = 1, 2$, solve the original NLP problem with bounds on p given by $\mathcal{R}_i$.
If a feasible solution $p_{\mathcal{R}_i}$ is obtained with objective function $J^u_{\mathcal{R}_i} < J^u$, then update the best feasible solution found so far $p^* := p_{\mathcal{R}_i}$, set $J^u := J^u_{\mathcal{R}_i}$ and remove from the list $\mathcal{L}$ all subregions $\mathcal{R}'$ such that $J^{\ell}_{\mathcal{R}'} > J^u$.

Step 8: Lower bound for each region

Obtain bounds on the differential variables.
If the α-based relaxation is additionally used for the overestimation of the equality constraints then obtain bounds on the second-order sensitivities.
Form the relaxed problem for each subregion $\mathcal{R}_1, \mathcal{R}_2$ and solve it.
For $i = 1, 2$, if a feasible solution $p^*_{\mathcal{R}_i}$ is obtained for $\mathcal{R}_i$ with objective function $J^{\ell}_{\mathcal{R}_i} \leqslant J^u$, then add $\mathcal{R}_i$ to the list $\mathcal{L}$ together with $J^{\ell}_{\mathcal{R}_i}$ and $p^*_{\mathcal{R}_i}$.
Go to step 4.

3.2.2. *Step 6: Branching*

The variable on which to branch is selected via one of the two strategies analyzed by Papamichail and Adjiman (2002).

3.2.3. *Step 7: Upper bound calculation*

To reduce the computational expense arising from the repeated solution of local dynamic optimization problems, the upper bound generation does not have to be applied at every iteration of the algorithm. This does not affect the ability of the algorithm to identify the global solution.

3.2.4. *Step 8: Lower bound calculation*

In the BB algorithm of Horst and Tuy (1996) if the relaxed problem is feasible then it has to be as tight as the relaxation at its parent node to ensure that the bounding operation is improving. A step to enforce this requirement was included in the algorithm presented by Papamichail and Adjiman (2002). However, in the following section it is shown that this is not necessary because of the theoretical properties of the underestimation strategy used.

4. Bound improvement

In this section, it is proved that the proposed selection operation is bound improving. To this effect, a key result is obtained for the proposed convex relaxation of the dynamic information: it is shown that partitioning of the parameter space results in a monotonically improving approximation of the objective function and feasible region.

THEOREM 4.1. *If natural interval extensions are used as inclusion functions and* $[p_2^L, p_2^U] \subset [p_1^L, p_1^U]$*, then the solution of the system*

$$\begin{aligned}
\dot{\underline{x}}_k(t) &= \inf f_k(t, \underline{x}_k(t), [\underline{x}_{k^-}(t), \overline{x}_{k^-}(t)], [p_1^L, p_1^U]) \\
\dot{\overline{x}}_k(t) &= \sup f_k(t, \overline{x}_k(t), [\underline{x}_{k^-}(t), \overline{x}_{k^-}(t)], [p_1^L, p_1^U]) \\
&\quad \forall t \in \mathcal{I} \quad \text{and} \quad k = 1, 2, \ldots, n
\end{aligned} \tag{15}$$

$$\begin{aligned}
\underline{x}(t_0) &= \inf x_0([p_1^L, p_1^U]) \\
\overline{x}(t_0) &= \sup x_0([p_1^L, p_1^U])
\end{aligned} \tag{16}$$

and the solution of the system

$$\begin{aligned}
\dot{\underline{\underline{x}}}_k(t) &= \inf f_k(t, \underline{\underline{x}}_k(t), [\underline{\underline{x}}_{k^-}(t), \overline{\overline{x}}_{k^-}(t)], [p_2^L, p_2^U]) \\
\dot{\overline{\overline{x}}}_k(t) &= \sup f_k(t, \overline{\overline{x}}_k(t), [\underline{\underline{x}}_{k^-}(t), \overline{\overline{x}}_{k^-}(t)], [p_2^L, p_2^U]) \\
&\quad \forall t \in \mathcal{I} \quad \text{and} \quad k = 1, 2, \ldots, n
\end{aligned} \tag{17}$$

$$\begin{aligned}
\underline{\underline{x}}(t_0) &= \inf x_0([p_2^L, p_2^U]) \\
\overline{\overline{x}}(t_0) &= \sup x_0([p_2^L, p_2^U])
\end{aligned} \tag{18}$$

are such that

$$\underline{x}(t) \leqslant \underline{\underline{x}}(t) \quad \forall t \in \mathcal{I} \tag{19}$$

and

$$\overline{\overline{x}}(t) \leqslant \overline{x}(t) \quad \forall t \in \mathcal{I}. \tag{20}$$

Proof. Using natural interval extensions as inclusion functions and the inclusion isotonicity property of interval operations the following is true:

$$\begin{aligned}[p_2^L, p_2^U] \subset [p_1^L, p_1^U] &\Rightarrow x_0([p_2^L, p_2^U]) \subseteq x_0([p_1^L, p_1^U]) \\ &\Rightarrow \begin{cases} \inf x_0([p_1^L, p_1^U]) \leqslant \inf x_0([p_2^L, p_2^U]) \\ \sup x_0([p_2^L, p_2^U]) \leqslant \sup x_0([p_1^L, p_1^U]) \end{cases}\end{aligned}$$

and using equations (16) and (18)

$$\underline{x}(t_0) \leqslant \underline{\underline{x}}(t_0) \tag{21}$$

and

$$\overline{\overline{x}}(t_0) \leqslant \overline{x}(t_0).$$

If one of the following:

$$\underline{x}(t) \leqslant \underline{\underline{x}}(t) \quad \forall t \in \mathcal{I}_0 \tag{22}$$

or

$$\overline{\overline{x}}(t) \leqslant \overline{x}(t) \quad \forall t \in \mathcal{I}_0$$

is not true then there exists $\xi_1 \in \mathcal{I}$ such that for some $k \in \{1, 2, \ldots, n\}$

$$\underline{x}_k(\xi_1) = \underline{\underline{x}}_k(\xi_1), \tag{23}$$

$$\dot{\underline{x}}_k(\xi_1) > \dot{\underline{\underline{x}}}_k(\xi_1) \tag{24}$$

and

$$\underline{x}(t) \leqslant \underline{\underline{x}}(t) \quad \forall t \in [0, \xi_1], \tag{25}$$

$$\overline{\overline{x}}(t) \leqslant \overline{x}(t) \quad \forall t \in [0, \xi_1] \tag{26}$$

or there exists $\xi_2 \in \mathcal{I}$ such that for some $k \in \{1, 2, \ldots, n\}$

$$\overline{x}_k(\xi_2) = \overline{\overline{x}}_k(\xi_2),$$

$$\dot{\overline{x}}_k(\xi_2) < \dot{\overline{\overline{x}}}_k(\xi_2)$$

and

$$\underline{x}(t) \leqslant \underline{\underline{x}}(t) \quad \forall t \in [0, \xi_2],$$
$$\overline{\overline{x}}(t) \leqslant \overline{x}(t) \quad \forall t \in [0, \xi_2].$$

Using equations (15) and (17) and inequality (24) the following must hold:

$$\begin{aligned} &\inf f_k(\xi_1, \underline{x}_k(\xi_1), [\underline{x}_{k^-}(\xi_1), \overline{x}_{k^-}(\xi_1)], [p_1^L, p_1^U]) \\ &> \inf f_k(\xi_1, \underline{\underline{x}}_k(\xi_1), [\underline{\underline{x}}_{k^-}(\xi_1), \overline{\overline{x}}_{k^-}(\xi_1)], [p_2^L, p_2^U]). \end{aligned} \tag{27}$$

However, based on the inclusion isotonicity property of interval operations and using equation (23), inequalities (25) and (26) and the relation $[p_2^L, p_2^U] \subset [p_1^L, p_1^U]$, inequality (27) is not true. This contradiction establishes the claim that inequality (22) is true and combined with inequality (21) it proves inequality (19).

In the same manner inequality (20) can be proved. □

LEMMA 4.1. *If* $\alpha_i^{(1)} \geqslant \alpha_i^{(2)} \geqslant 0,\ i = 1, 2, \ldots, m,$ then $\forall z \in [z_2^L, z_2^U] \subseteq [z_1^L, z_1^U] \subset \Re^m$*:*

$$\sum_{i=1}^{m} \alpha_i^{(1)} (z_{1,i}^L - z_i)(z_{1,i}^U - z_i) \leqslant \sum_{i=1}^{m} \alpha_i^{(2)} (z_{2,i}^L - z_i)(z_{2,i}^U - z_i).$$

Proof. Let $z \in [z_2^L, z_2^U] \subseteq [z_1^L, z_1^U] \subset \Re^m$. Then

$$(z_{1,i}^L - z_i)(z_{1,i}^U - z_i) \leqslant (z_{2,i}^L - z_i)(z_{2,i}^U - z_i) \leqslant 0,\ i = 1, 2, \ldots, m.$$

If $\alpha_i^{(1)} \geqslant \alpha_i^{(2)} \geqslant 0,\ i = 1, 2, \ldots, m,$ then

$$\alpha_i^{(1)} (z_{1,i}^L - z_i)(z_{1,i}^U - z_i) \leqslant \alpha_i^{(2)} (z_{2,i}^L - z_i)(z_{2,i}^U - z_i) \leqslant 0,\ i = 1, 2, \ldots, m$$

and consequently $\forall z \in [z_2^L, z_2^U] \subseteq [z_1^L, z_1^U] \subset \Re^m$

$$\sum_{i=1}^{m} \alpha_i^{(1)} (z_{1,i}^L - z_i)(z_{1,i}^U - z_i) \leqslant \sum_{i=1}^{m} \alpha_i^{(2)} (z_{2,i}^L - z_i)(z_{2,i}^U - z_i). \qquad \square$$

LEMMA 4.2. *Let the symmetric interval matrices* $[H_1]$ *and* $[H_2]$ *be defined such that* $[H_1] = ([\underline{h}_{ij}^{(1)}, \overline{h}_{ij}^{(1)}])$ *and* $[H_2] = ([\underline{h}_{ij}^{(2)}, \overline{h}_{ij}^{(2)}])$*. For any vector* $d^{(1)} > 0$ *let* $\alpha_i^{(1)}$ *be calculated by*

$$\alpha_i^{(1)} = \max \left\{ 0, -\frac{1}{2} \left(\underline{h}_{ii}^{(1)} - \sum_{j \neq i} |h|_{ij}^{(1)} \frac{d_j^{(1)}}{d_i^{(1)}} \right) \right\}, \tag{28}$$

where $|h|_{ij}^{(1)} = \max\{|\underline{h}_{ij}^{(1)}|, |\overline{h}_{ij}^{(1)}|\}$ *and for any vector* $d^{(2)} > 0$ *let* $\alpha_i^{(2)}$ *be calculated by*

$$\alpha_i^{(2)} = \max\left\{0, -\frac{1}{2}\left(\underline{h}_{ii}^{(2)} - \sum_{j\neq i}|h|_{ij}^{(2)}\frac{d_j^{(2)}}{d_i^{(2)}}\right)\right\}, \tag{29}$$

where $|h|_{ij}^{(2)} = \max\{|\underline{h}_{ij}^{(2)}|, |\overline{h}_{ij}^{(2)}|\}$. *If* $d^{(1)} = d^{(2)} = d$ *is a constant vector and* $[H_2] \subseteq [H_1]$, *then* $\alpha_i^{(1)} \geqslant \alpha_i^{(2)}$.

Proof. If $[H_2] \subseteq [H_1]$, then from the definition of these interval matrices the following can be derived:

$$\underline{h}_{ij}^{(1)} \leqslant \underline{h}_{ij}^{(2)} \text{ and } \overline{h}_{ij}^{(2)} \leqslant \overline{h}_{ij}^{(1)}. \tag{30}$$

Therefore,

$$|h|_{ij}^{(1)} = \max\{|\underline{h}_{ij}^{(1)}|, |\overline{h}_{ij}^{(1)}|\} \geqslant \max\{|\underline{h}_{ij}^{(2)}|, |\overline{h}_{ij}^{(2)}|\} = |h|_{ij}^{(2)}.$$

Hence, for any $d^{(1)} = d^{(2)} = d > 0$

$$\sum_{j\neq i}|h|_{ij}^{(1)}\frac{d_j}{d_i} \geqslant \sum_{j\neq i}|h|_{ij}^{(2)}\frac{d_j}{d_i}. \tag{31}$$

From inequalities (30) and (31), it follows that

$$-\frac{1}{2}\left(\underline{h}_{ii}^{(1)} - \sum_{j\neq i}|h|_{ij}^{(1)}\frac{d_j}{d_i}\right) \geqslant -\frac{1}{2}\left(\underline{h}_{ii}^{(2)} - \sum_{j\neq i}|h|_{ij}^{(2)}\frac{d_j}{d_i}\right).$$

Therefore,

$$\max\left\{0, -\frac{1}{2}\left(\underline{h}_{ii}^{(1)} - \sum_{j\neq i}|h|_{ij}^{(1)}\frac{d_j}{d_i}\right)\right\} \geqslant \max\left\{0, -\frac{1}{2}\left(\underline{h}_{ii}^{(2)} - \sum_{j\neq i}|h|_{ij}^{(2)}\frac{d_j}{d_i}\right)\right\}$$

and from (28) and (29) it follows that $\alpha_i^{(1)} \geqslant \alpha_i^{(2)}$. □

LEMMA 4.3. *Let*

$$\breve{f}_{NT}^{(1)}(z) = f_{NT}(z) + \sum_{i=1}^{m}\alpha_i^{(1)}(z_{1,i}^L - z_i)(z_{1,i}^U - z_i) \tag{32}$$

and

$$\breve{f}_{NT}^{(2)}(z) = f_{NT}(z) + \sum_{i=1}^{m} \alpha_i^{(2)}(z_{2,i}^L - z_i)(z_{2,i}^U - z_i) \tag{33}$$

be the α*-based convex underestimators of the general nonconvex twice continuously differentiable function* $f_{NT}(z)$ *over the domains* $[z_1^L, z_1^U] \subset \Re^m$ *and* $[z_2^L, z_2^U] \subset \Re^m$*, respectively. Let the scaled Gerschgorin method, with constant vector* $d > 0$*, proposed by Adjiman et al. (1998b) be used for the calculation of all the non-negative* $\alpha_i^{(1)}$ *and* $\alpha_i^{(2)}$ *parameters and let* $[H_1] = ([\underline{h}_{ij}^{(1)}, \overline{h}_{ij}^{(1)}]) \ni H_{f_{NT}}(z) = \nabla^2 f_{NT}(z)\ \forall z \in [z_1^L, z_1^U]$ *and* $[H_2] = ([\underline{h}_{ij}^{(2)}, \overline{h}_{ij}^{(2)}]) \ni H_{f_{NT}}(z) = \nabla^2 f_{NT}(z)$ $\forall z \in [z_2^L, z_2^U]$ *be the interval matrices needed. If* $[z_2^L, z_2^U] \subseteq [z_1^L, z_1^U]$ *and* $[H_2] \subseteq [H_1]$*, then* $\breve{f}_{NT}^{(1)}(z) \leqslant \breve{f}_{NT}^{(2)}(z)\ \forall z \in [z_2^L, z_2^U]$.

Proof. If the scaled Gerschgorin method proposed by Adjiman et al. (1998b) is used for the calculation of all the non-negative $\alpha_i^{(1)}$ and $\alpha_i^{(2)}$ parameters, then these can be given by equations (28) and (29). If $d^{(1)} = d^{(2)} = d > 0$ is a constant vector and $[H_2] \subseteq [H_1]$ then using Lemma 4.2 it is proved that

$$\alpha_i^{(1)} \geqslant \alpha_i^{(2)}.$$

Therefore, using Lemma 4.1 $\forall z \in [z_2^L, z_2^U] \subseteq [z_1^L, z_1^U] \subset \Re^m$ the following is true:

$$\sum_{i=1}^{m} \alpha_i^{(1)}(z_{1,i}^L - z_i)(z_{1,i}^U - z_i) \leqslant \sum_{i=1}^{m} \alpha_i^{(2)}(z_{2,i}^L - z_i)(z_{2,i}^U - z_i)$$

and using equations (32) and (33) $\breve{f}_{NT}^{(1)}(z) \leqslant \breve{f}_{NT}^{(2)}(z)\ \forall z \in [z_2^L, z_2^U]$. □

LEMMA 4.4. *Let* $[H_1] = ([\underline{h}_{ij}^{(1)}, \overline{h}_{ij}^{(1)}]) \ni H_{f_{NT}}(z) = \nabla^2 f_{NT}(z)\ \forall z \in [z_1^L, z_1^U]$ *and* $[H_2] = ([\underline{h}_{ij}^{(2)}, \overline{h}_{ij}^{(2)}]) \ni H_{f_{NT}}(z) = \nabla^2 f_{NT}(z)\ \forall z \in [z_2^L, z_2^U]$*. If the method described in Section* 3.1.2 *is used for the derivation of* α*-based convex underestimators of the general nonconvex twice continuously differentiable term* $f_{NT}(z)$ *and* $[z_2^L, z_2^U] \subseteq [z_1^L, z_1^U] \subset \Re^m$ *then* $[H_2] \subseteq [H_1]$.

Proof. If the method described in Section 3.1.2 is used for the derivation of α-based convex underestimators of the general nonconvex twice continuously differentiable term $f_{NT}(z)$ then natural interval extensions are used as inclusion functions. If $[z_2^L, z_2^U] \subseteq [z_1^L, z_1^U] \subset \Re^m$ then based on the inclusion isotonicity property of interval operations $[H_2] \subseteq [H_1]$. □

LEMMA 4.5. *Let* $[H_1] \ni H_{x_k(t_i)}(p) = \nabla^2 x_k(t_i, p)\ \forall p \in [p_1^L, p_1^U]$ *and* $[H_2] \ni H_{x_k(t_i)}(p) = \nabla^2 x_k(t_i, p)\ \forall p \in [p_2^L, p_2^U]$*. Let also* $[H_3] \ni H_{x_k^-(t_i)}(p) = \nabla^2 x_k^-(t_i, p)$

$\forall p \in [p_1^L, p_1^U]$ *and* $[H_4] \ni H_{x_k^-(t_i)}(p) = \nabla^2 x_k^-(t_i, p)$ $\forall p \in [p_2^L, p_2^U]$. *If the method described in Section* 3.1.3 *is used for the derivation of* α*-based convex underestimators of the general nonconvex twice continuously differentiable functions* $x_k(t_i, p)$ *and* $x_k^-(t_i, p)$ *and* $[p_2^L, p_2^U] \subset [p_1^L, p_1^U] \subset \Re^r$ *then* $[H_2] \subseteq [H_1]$ *and* $[H_4] \subseteq [H_3]$.

Proof. If the method described in Section 3.1.3 is used for the derivation of α-based convex underestimators of the general nonconvex twice continuously differentiable functions $x_k(t_i, p)$ and $[p_2^L, p_2^U] \subset [p_1^L, p_1^U]$ then using Theorem 4.1 $[H_2] \subseteq [H_1]$. In the same manner $[H_4] \subseteq [H_3]$. □

LEMMA 4.6. *If the convex envelope* $c_{\mathcal{R}}(f(z))$ *is used for the convex underestimation of a function* $f(z)$ *over the domain* $\mathcal{R}$ *then* $c_{\mathcal{R}}(f(z)) \leqslant c_{\mathcal{R}'}(f(z))$ $\forall z \in \mathcal{R}' \subseteq \mathcal{R}$.

Proof. The proof is derived easily from the definition of convex envelopes (Falk and Soland, 1969). □

THEOREM 4.2. *Let the method described in Section* 3.1 *be used for the construction of the convex relaxation of the original NLP problem (1). If the relaxed problem is feasible on* $\mathcal{R}'$, *then* $J_{\mathcal{R}}^l \leqslant J_{\mathcal{R}'}^l$ $\forall p \in \mathcal{R}' \subset \mathcal{R}$. *This means that the lower bound calculated at a node of the spatial BB algorithm is at least as tight as that of the parent node.*

Proof. If the relaxed problem is feasible on $\mathcal{R}'$, then $J_{\mathcal{R}}^l \leqslant J_{\mathcal{R}'}^l$ $\forall p \in \mathcal{R}' \subset \mathcal{R}$ is implied if the feasible region of the relaxed problem derived on $\mathcal{R}'$ is at least as tight as that derived on $\mathcal{R}$ $\forall p \in \mathcal{R}'$ and the objective function of the relaxed problem derived on $\mathcal{R}'$ is at least as tight as that derived on $\mathcal{R}$ $\forall p \in \mathcal{R}'$.

If the method described in Section 3.1 is used for the calculation of constant bounds on the variables $\hat{x}_i$, $i = 0, 1, \ldots, NS$, then based on Theorem 4.1 the bounds derived on $\mathcal{R}'$ are at least as tight as those derived on $\mathcal{R}$ $\forall p \in \mathcal{R}'$.

The convex relaxation of the bilinear terms is derived using the convex envelope proposed by McCormick (1976). Based on the previous statement and Lemma 4.6 the relaxation of a bilinear term derived on $\mathcal{R}'$ is at least as tight as that derived on $\mathcal{R}$ $\forall p \in \mathcal{R}'$.

The convex underestimation of the functions g_{ij}, $i = 0, 1, \ldots, NS$, $j = 1, 2, \ldots, s_i$ derived on $\mathcal{R}'$ is at least as tight as that derived on $\mathcal{R}$ $\forall p \in \mathcal{R}'$ if the same is true for the convex relaxation of univariate concave terms and general nonconvex twice continuously differentiable terms. The convex envelope is used for the underestimation of univariate concave terms and by using Lemma 4.6 the required property can be shown. For the convex underestimation of general nonconvex twice continuously differentiable terms the α-based convex underestimator is used and based on Lemmas 4.4 and 4.3 the required property can be shown.

If the α-based method is additionally used for the convex relaxation of the set of equality constraints then based on Lemmas 4.5 and 4.3 the relaxation derived on $\mathcal{R}'$ is at least as tight as that derived on $\mathcal{R}$ $\forall p \in \mathcal{R}'$.

Using all the previous statements it is shown that the feasible region of the relaxed problem derived on $\mathcal{R}'$ is at least as tight as that derived on $\mathcal{R}$ $\forall p \in \mathcal{R}'$.

The required property for the objective function of the relaxed problem can be shown if the analysis followed for the functions g_{ij}, $i = 0, 1, \ldots, NS$, $j = 1, 2, \ldots, s_i$ is also followed for the function J. □

Remark 4.1. The scaled Gerschgorin method proposed by Adjiman et al. (1998b) requires the use of a vector $d > 0$. In the algorithm presented in Section 3 a constant d is used. If d varies as branching occurs then at Step 8 of the algorithm the value of each α has to be less than or equal to its value at the parent node so as to guarantee bound improvement. If this is not true, then the value at the parent node can be used as it is a valid one.

DEFINITION 4.1 (IV.6 in Horst and Tuy, 1996). A selection operation is said to be bound improving if, at least each time after a finite number of iterations at least one partition element where the actual bound is attained is selected for further partition.

LEMMA 4.7. *The selection operation in the BB algorithm presented in Section 3 is bound improving.*

Proof. In Step 4 of the BB algorithm presented in Section 3 the region where the actual bound is attained is selected for further partition. Hence, the selection operation is bound improving based on Definition 4.1. □

5. Consistency of the bounding operation

In this section, it is proved that the proposed bounding operation is consistent. For this purpose, it is shown that the convex relaxation of the dynamic information coincides with the original dynamic variables in the limit of partitioning. Similar properties are derived for the convex relaxation of the nonconvex terms.

DEFINITION 5.1 (IV.4 in Horst and Tuy, 1996). A bounding operation is called consistent if at every step any unfathomed partition element can be further refined, and if any infinitely decreasing sequence $\{\mathcal{R}_{Iter_q}\}$ of successively refined partition elements satisfies:

$$\lim_{q\to\infty}(J^u_{Iter_q} - J^l_{\mathcal{R}_{Iterq}}) = 0.$$

The last relation will be implied by the most practical requirement:

$$\lim_{q\to\infty}(J^u_{\mathcal{R}_{Iterq}} - J^l_{\mathcal{R}_{Iterq}}) = 0, \tag{34}$$

which simply states that, whenever a decreasing sequence of partition sets converges to a certain limit set, the bounds also must converge to the exact minimum of J over this limit set.

LEMMA 5.1. *Let $\varepsilon \geqslant 0$ be a finite number such that $||p^U - p^L|| \leqslant \varepsilon$, where $||\cdot||$ is the* max *norm. If there exists a finite number $\lambda \geqslant 0$ such that for $t_1 \in \mathcal{I}$ $||\overline{x}(t_1) - \underline{x}(t_1)|| \leqslant \lambda\varepsilon$ then there exists a finite number $\nu \geqslant 0$ such that*

$$||\overline{x}(t) - \underline{x}(t)|| \leqslant \nu\varepsilon \ \forall t \in \mathcal{I},\ t \geqslant t_1,$$

where $\overline{x}(t)$ and $\underline{x}(t)$ $\forall t \in \mathcal{I}$ are given by the solution of the system

$$\begin{aligned} \dot{\underline{x}}_k(t) &= \inf f_k(t, \underline{x}_k(t), [\underline{x}_{k^-}(t), \overline{x}_{k^-}(t)], [p^L, p^U]) \\ \dot{\overline{x}}_k(t) &= \sup f_k(t, \overline{x}_k(t), [\underline{x}_{k^-}(t), \overline{x}_{k^-}(t)], [p^L, p^U]) \\ &\forall t \in \mathcal{I} \quad \text{and} \quad k = 1, 2, \ldots, n \end{aligned} \tag{35}$$

$$\begin{aligned} \underline{x}(t_0) &= \inf x_0([p^L, p^U]) \\ \overline{x}(t_0) &= \sup x_0([p^L, p^U]) \end{aligned} \tag{36}$$

f is a continuous function and natural interval extensions are used as inclusion functions.

Proof. Using equations (35), natural interval extensions as inclusion functions and the inclusion isotonicity property of interval operations the following are true:

$$\begin{aligned} ||\dot{\overline{x}}(t_2) - \dot{\underline{x}}(t_2)|| &= \max_{k=1}^{n}\{\dot{\overline{x}}_k(t_2) - \dot{\underline{x}}_k(t_2)\} \\ &= \max_{k=1}^{n}\{\sup f_k(t_2, \overline{x}_k(t_2), [\underline{x}_{k^-}(t_2), \overline{x}_{k^-}(t_2)], [p^L, p^U]) \\ &\quad - \inf f_k(t_2, \underline{x}_k(t_2), [\underline{x}_{k^-}(t_2), \overline{x}_{k^-}(t_2)], [p^L, p^U])\} \end{aligned}$$

$$\begin{aligned}
&\leqslant \max_{k=1}^{n}\{\sup f_k(t_2,[\underline{x}(t_2),\overline{x}(t_2)],[p^L,p^U])\\
&\quad -\inf f_k(t_2,[\underline{x}(t_2),\overline{x}(t_2)],[p^L,p^U])\}\\
&=\max_{k=1}^{n} w(f_k(t_2,[\underline{x}(t_2),\overline{x}(t_2)],[p^L,p^U]))\\
&=w(f(t_2,[\underline{x}(t_2),\overline{x}(t_2)],[p^L,p^U]))
\end{aligned}$$

where $w(\cdot)$ is the width of an interval. Therefore, if $\varepsilon \geqslant 0$ is a finite number such that $||p^U - p^L|| \leqslant \varepsilon$ and there exists a finite number $\mu \geqslant 0$ such that for $t_2 \in \mathcal{I}$ $||\overline{x}(t_2) - \underline{x}(t_2)|| \leqslant \mu\varepsilon$, then there exists a finite number $\kappa \geqslant 0$ such that

$$||\dot{\overline{x}}(t_2) - \dot{\underline{x}}(t_2)|| \leqslant \kappa\varepsilon.$$

For $t_3 = t_2 + \Delta t$, $\Delta t > 0$ the following is true:

$$\begin{aligned}
\lim_{\Delta t\to 0} ||\overline{x}(t_3) - \underline{x}(t_3)|| &= \lim_{\Delta t\to 0} ||\overline{x}(t_2) - \underline{x}(t_2) + (\dot{\overline{x}}(t_2) - \dot{\underline{x}}(t_2))\,\Delta t||\\
&\leqslant ||\overline{x}(t_2) - \underline{x}(t_2)|| + \lim_{\Delta t\to 0} ||\dot{\overline{x}}(t_2) - \dot{\underline{x}}(t_2)||\,\Delta t\\
&\leqslant \mu\varepsilon + \kappa\varepsilon \lim_{\Delta t\to 0} \Delta t = \mu\varepsilon + 0 = \mu\varepsilon,
\end{aligned}$$

Hence,

$$\lim_{\Delta t\to 0} ||\overline{x}(t_3) - \underline{x}(t_3)|| \leqslant \mu\varepsilon.$$

Based on the latter statements and the fact that there exists a finite number $\lambda \geqslant 0$ such that for $t_1 \in \mathcal{I}$ $||\overline{x}(t_1) - \underline{x}(t_1)|| \leqslant \lambda\varepsilon$, there also exists a finite number $\nu \geqslant 0$ such that

$$||\overline{x}(t) - \underline{x}(t)|| \leqslant \nu\varepsilon \;\forall t \in \mathcal{I},\; t \geqslant t_1. \qquad \square$$

LEMMA 5.2. *If f and x_0 are continuous and natural interval extensions are used as inclusion functions, then the solution of the system:*

$$\begin{aligned}
&\dot{\underline{x}}_k(t) = \inf f_k(t,\underline{x}_k(t),[\underline{x}_{k^-}(t),\overline{x}_{k^-}(t)],[p^L,p^U])\\
&\dot{\overline{x}}_k(t) = \sup f_k(t,\overline{x}_k(t),[\underline{x}_{k^-}(t),\overline{x}_{k^-}(t)],[p^L,p^U])\\
&\qquad \forall t \in \mathcal{I} \quad \text{and} \quad k = 1,2,\ldots,n
\end{aligned} \tag{37}$$

$$\begin{aligned}
&\underline{x}(t_0) = \inf x_0([p^L,p^U])\\
&\overline{x}(t_0) = \sup x_0([p^L,p^U])
\end{aligned} \tag{38}$$

is such that

$$\lim_{||p^U - p^L|| \to 0} (\overline{x}_k(t) - \underline{x}_k(t)) = 0 \quad \forall t \in \mathcal{I},\ k = 1, 2, \ldots, n.$$

Proof. Let $\varepsilon \geqslant 0$ be a finite number such that $||p^U - p^L|| \leqslant \varepsilon$. Using equations (38) there exists a finite number $\lambda \geqslant 0$ such that

$$\begin{aligned} ||\overline{x}(t_0) - \underline{x}(t_0)|| &= ||\sup x_0([p^L, p^U]) - \inf x_0([p^L, p^U])|| \\ &= w(x_0([p^L, p^U])) \leqslant \lambda\varepsilon. \end{aligned}$$

If natural interval extensions are used as inclusion functions then from Lemma 5.1 it can be proved that there exists a finite number $\nu \geqslant 0$ such that

$$||\overline{x}(t) - \underline{x}(t)|| \leqslant \nu\varepsilon \ \forall t \in \mathcal{I},$$

where $\overline{x}(t)$ and $\underline{x}(t)$ $\forall t \in \mathcal{I}$ are given by the solution of system (37)–(38). Therefore $\forall t \in \mathcal{I}$, $k = 1, 2, \ldots, n$ the following is true:

$$\begin{aligned} 0 \leqslant \lim_{||p^U - p^L|| \to 0} (\overline{x}_k(t) - \underline{x}_k(t)) &\leqslant \lim_{||p^U - p^L|| \to 0} ||\overline{x}(t) - \underline{x}(t)|| \\ &= \lim_{\varepsilon \to 0} ||\overline{x}(t) - \underline{x}(t)|| \leqslant \lim_{\varepsilon \to 0} \nu\varepsilon = 0. \end{aligned}$$

Hence,

$$\lim_{||p^U - p^L|| \to 0} (\overline{x}_k(t) - \underline{x}_k(t)) = 0 \quad \forall t \in \mathcal{I},\ k = 1, 2, \ldots, n. \qquad \square$$

LEMMA 5.3. *Let $z \in \Re^m$ and $i,\ j \in \{1, 2, \ldots, m\}$ and let*

$$Z(z) = \{z_i z_j - \max(z_i^L z_j + z_i z_j^L - z_i^L z_j^L, z_i^U z_j + z_i z_j^U - z_i^U z_j^U)\}.$$

The following is always true:

$$\lim_{||z^U - z^L|| \to 0} \max_{z \in [z^L, z^U]} Z(z) = 0.$$

Proof. The following has been proved by Androulakis et al. (1995):

$$\max_{z \in [z^L, z^U]} Z(z) = \frac{(z_i^U - z_i^L)(z_j^U - z_j^L)}{4}$$

and therefore,

$$\lim_{||z^U - z^L|| \to 0} \max_{z \in [z^L, z^U]} Z(z) = \lim_{||z^U - z^L|| \to 0} \frac{(z_i^U - z_i^L)(z_j^U - z_j^L)}{4} = 0. \qquad \square$$

LEMMA 5.4. *Let*

$$\breve{f}_{NT}(z) = f_{NT}(z) + \sum_{i=1}^{m} \alpha_i (z_i^L - z_i)(z_i^U - z_i),$$

where $z \in [z^L, z^U] \subset \Re^m$. *The following is always true:*

$$\lim_{||z^U - z^L|| \to 0} \max_{z \in [z^L, z^U]} (f_{NT}(z) - \breve{f}_{NT}(z)) = 0.$$

Proof. The following has been proved by Androulakis et al. (1995):

$$\max_{z \in [z^L, z^U]} (f_{NT}(z) - \breve{f}_{NT}(z)) = \frac{1}{4} \sum_{i=1}^{m} \alpha_i (z_i^U - z_i^L)^2$$

and therefore,

$$\lim_{||z^U - z^L|| \to 0} \max_{z \in [z^L, z^U]} (f_{NT}(z) - \breve{f}_{NT}(z))$$

$$= \lim_{||z^U - z^L|| \to 0} \frac{1}{4} \sum_{i=1}^{m} \alpha_i (z_i^U - z_i^L)^2 = 0. \qquad \square$$

LEMMA 5.5. *Let* $f_{UT}(z)$ *be a univariate concave function, where* $z \in \Re$. *If* $\breve{f}_{UT}(z)$ *is the secant underestimator over the domain* $[z^L, z^U] \subset \Re$, *then*

$$\lim_{||z^U - z^L|| \to 0} \max_{z \in [z^L, z^U]} (f_{UT}(z) - \breve{f}_{UT}(z)) = 0.$$

Proof. The secant underestimator is the convex envelope of a univariate concave term, which means that it is the tightest possible convex underestimator. If $\breve{f}_{\alpha}(z)$ is the α-based underestimator (Maranas and Floudas, 1994; Androulakis et al., 1995) of $f_{UT}(z)$ over the domain $[z^L, z^U] \subset \Re$, then

$$\max_{z \in [z^L, z^U]} (f_{UT}(z) - \breve{f}_{UT}(z)) \leqslant \max_{z \in [z^L, z^U]} (f_{UT}(z) - \breve{f}_{\alpha}(z)) = \frac{1}{4} \alpha (z^U - z^L)^2$$

and therefore,

$$0 \leqslant \lim_{||z^U - z^L|| \to 0} \max_{z \in [z^L, z^U]} (f_{UT}(z) - \breve{f}_{UT}(z)) \leqslant \lim_{||z^U - z^L|| \to 0} \frac{1}{4} \alpha (z^U - z^L)^2.$$

Since $\lim_{||z^U - z^L|| \to 0} \frac{1}{4} \alpha (z^U - z^L)^2 = 0$,

$$\lim_{||z^U - z^L|| \to 0} \max_{z \in [z^L, z^U]} (f_{UT}(z) - \breve{f}_{UT}(z)) = 0. \qquad \square$$

LEMMA 5.6. *Let* $A(z):\Re^m \mapsto \Re$ *and* $B(z):\Re^m \mapsto \Re$. *Let also* $A(z) \geqslant 0$ *and* $B(z) \geqslant 0$ $\forall z \in [z^L, z^U] \subset \Re^m$ *and*

$$\lim_{||z^U - z^L|| \to 0} \max_{z \in [z^L, z^U]} A(z) = \lim_{||z^U - z^L|| \to 0} \max_{z \in [z^L, z^U]} B(z) = 0.$$

Then

$$\lim_{||z^U - z^L|| \to 0} \max_{z \in [z^L, z^U]} \{A(z) + B(z)\} = 0.$$

Proof. If $A(z) \geqslant 0$ and $B(z) \geqslant 0 \quad \forall z \in [z^L, z^U]$ then

$$0 \leqslant \max_{z \in [z^L, z^U]} \{A(z) + B(z)\} \leqslant \max_{z \in [z^L, z^U]} \{A(z)\} + \max_{z \in [z^L, z^U]} \{B(z)\}$$

and therefore,

$$0 \leqslant \lim_{||z^U - z^L|| \to 0} \max_{z \in [z^L, z^U]} \{A(z) + B(z)\}$$
$$= \lim_{||z^U - z^L|| \to 0} \max_{z \in [z^L, z^U]} A(z) + \lim_{||z^U - z^L|| \to 0} \max_{z \in [z^L, z^U]} B(z) = 0.$$

Hence,

$$\lim_{||z^U - z^L|| \to 0} \max_{z \in [z^L, z^U]} \{A(z) + B(z)\} = 0.$$ □

THEOREM 5.1. *The bounding operation in the BB algorithm presented in Section 3 is consistent.*

Proof. Based on Definition 5.1 and the most practical requirement (34) a bounding operation is called consistent if at every step any unfathomed partition element can be further refined and whenever a decreasing sequence of partition sets converges to a certain limit set, the bounds also converge to the exact minimum of J over this limit set. The first requirement is true for the BB algorithm presented in Section 3. The second requirement is implied if whenever a decreasing sequence of partition sets converges to a certain limit set, the maximum distances between the constraints and their convex relaxation and the maximum distance between the objective function and its convex underestimation converge to zero.

Based on Lemma 5.2 the latter requirement is true for the equality constraints and based on Lemma 5.3 the same is true for the relaxation of the bilinear terms. The distances between the functions g_{ij}, $i = 0, 1, \ldots, NS$, $j = 1, 2, \ldots, s_i$ and their convex relaxation is a summation of the distances between the univariate concave terms and their convex underestimator and the distances between the general nonconvex twice continuously differentiable terms and their convex underestimator. Based on Lemmas 5.4, 5.5 and 5.6 whenever a decreasing sequence of partition sets converges to a certain limit set, the maximum distances converge to zero.

The required property for the maximum distance between the objective function and its convex underestimation can be shown if the analysis followed for the functions g_{ij}, $i=0,1,\dots,NS$, $j=1,2,\dots,s_i$ is also followed for the function J. □

6. Convergence of the spatial BB algorithm

THEOREM 6.1 (IV.3 in Horst and Tuy, 1996). *In the infinite BB procedure, suppose that the bounding operation is consistent and the selection operation is bound improving. Then the procedure is convergent.*

COROLLARY 6.1. *The BB algorithm presented in Section 3 converges to the global minimum of the original problem if $MaxIter$ is set to ∞ and ϵ_r is set to* 0.

Proof. If $MaxIter=\infty$ and $\epsilon_r=0$, then the BB algorithm presented in Section 3 is an infinite BB procedure and follows the one by Horst and Tuy (1996). The selection operation is bound improving based on Lemma 4.7. The bounding operation is consistent based on Theorem 5.1. From Theorem 6.1, it is deduced that the BB algorithm is a convergent procedure. □

7. Conclusions

Most of the existing algorithms for the optimization of systems which are described by ODEs can produce only local optimum solutions that can be used as an upper bound for the global optimum. A deterministic spatial BB global optimization algorithm for problem with ODEs in the constraints was developed by Papamichail and Adjiman (2002). Well known techniques were used for the required convex relaxation of bilinear terms, univariate concave terms and general nonconvex twice continuously differentiable terms.

The proof of convergence for this algorithm has been presented here. It is based on a bound improving selection operation and a consistent bounding operation. This proof is valid for any BB algorithm which follows the algorithm of Horst and Tuy (1996) and is applied to an NLP problem involving a subset of the nonconvex terms discussed in this work.

Acknowledgement

Financial support (GR/R52312/01) from the Engineering and Physical Sciences Research Council (EPSRC) is gratefully acknowledged.

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