Journal of Global Optimization, **30:** 59–89, 2004.

Global Optimization Issues in Multiparametric Continuous and Mixed-Integer Optimization Problems

V. DUA[1], K.P. PAPALEXANDRI[2] and E.N. PISTIKOPOULOS[1,*]
[1] *Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College, London SW7 2BY, U.K.*
[2] *BP Exploration, Research and Engineering Centre, U.K.*

(Received 28 March 2002; accepted in revised form 4 June 2003)

Abstract. In this paper, a number of theoretical and algorithmic issues concerning the solution of parametric nonconvex programs are presented. In particular, the need for defining a suitable overestimating subproblem is discussed in detail. The multiparametric case is also addressed, and a branch and bound (B&B) algorithm for the solution of parametric nonconvex programs is proposed.

Key words: Parametric global optimization, Parametric overestimators, Parametric nonconvex programming

1. Introduction, Background and Motivation

Consider the following nonconvex program:

$$z = \min_x f(x) \tag{1.1}$$

$$\text{s.t.} \quad g_i(x) \leqslant 0, i = 1, \dots, I \tag{1.2}$$

$$x_j^L \leqslant x_j \leqslant x_j^U, j = 1, \dots, J \tag{1.3}$$

$$x \in \Re^J, \tag{1.4}$$

where x is a vector of continuous variables, f is a scalar function, $g_i \leqslant 0, i = 1, \dots, I$ is the set of inequality constraints, and the superscripts L and U denote lower and upper bounds respectively. Many algorithms have been proposed for the global solution of (1) [18, 21, 27, 43]. While solution techniques based upon stochastic search, genetic algorithms and simulated annealing have been presented in the open literature (see [6] for references), in this work the focus is on deterministic optimization based algorithms. Note that the solution of (1) is quite important in the fields of science and engineering [22, 25]. Branch and bound (B&B) algorithms are amongst the most popular deterministic optimization algorithms.

*Author to whom correspondence should be addressed. E-mail: e.pistikopoulos@ic.ac.uk, Tel: +442075946620, Fax: +442075946606

Note that deterministic algorithms which are based upon duality theory, are also available [23]. B&B algorithms rely on obtaining upper and lower bounds on the solution of (1) which converge within a given tolerance as the iterative steps in the algorithm are taken [5]. An upper bound can be obtained by solving (1) by using a local optimizer. The lower bound is obtained by replacing all the nonconvex terms in f and g by the corresponding convex underestimators and then solving the resulting problem. Note that smaller the range of x, $[x^L, x^U]$, the tighter is the underestimator and hence tighter is the lower bound. In the next step, known as the branching of the B&B tree, for some x_j, the interval $[x_j^L, x_j^U]$ is partitioned into, say two, smaller intervals: $[x_j^L, x_j^{\otimes}]$ and $[x_j^{\otimes}, x_j^U]$ where $x_j^L < x_j^{\otimes} < x_j^U$. In the partitioned intervals the tighter underestimators are obtained and the corresponding underestimating subproblems are solved. The upper bound can also be tightened by solving (1) by using local optimization solvers in the partitioned intervals and then taking the lowest of all the values of these local optimal solutions and the upper bound obtained before partitioning. Note that the tightening of the lower bound means an increase in its value and for the upper bound a decrease in its value. The partitioned intervals where a solution of the underestimating subproblem is greater than or within a certain tolerance of the upper bound are removed from further consideration – this is known as bounding or fathoming. The remaining partitioned intervals are further partitioned into smaller intervals and this procedure continues until all the intervals except the ones where the global solution lies and is within a certain tolerance of the upper bound, have been fathomed. The partitioning or branching may take place for a different x_j at each iteration. Note the following two remarks regarding this solution approach.

REMARK 1. Solution of (1) by using a local optimizer provides an upper bound.

REMARK 2. For the solution of (1), fathoming of the partitioned sub-spaces is achieved by comparing lower and upper bounds which are simple numerical values.

In this paper we are concerned with the following parametric non-convex program:

$$z(\theta) = \min_x f(x) \tag{2.1}$$

$$\text{s.t.} \quad g_i(x) \leqslant b_i + F_i\theta, \quad i = 1, \dots, I \tag{2.2}$$

$$x_j^L \leqslant x_j \leqslant x_j^U, \quad j = 1, \dots, J \tag{2.3}$$

$$x \in \Re^J \tag{2.4}$$

$$\theta \in \Theta \subseteq \Re^S, \tag{2.5}$$

where θ is a vector of parameters and Θ is a compact and polyhedral convex set, b_i is the ith row of I dimensional constant column vector b and F_i is the

ith row of constant matrix F of dimension $I \times S$. The objectives is to obtain the complete profile of all the global solutions for all the values of $\theta \in \Theta$ without solving the global optimization problems for all the values of θ. Note that the assumptions that θ appears only on the right hand side of the constraints and that Θ is a convex set are not restrictive. For a given problem when these assumptions are not valid, then that problem can be reformulated as (2) by defining some additional variables, x, equal to the θs that violate the assumptions.

Computational requirements for finding the solution of (1) for a general case, and that of (2) even for the case when f and g are linear are not bounded by a polynomial in the size of the problem. Nevertheless the solution of (2) has immense practical applications: (i) hybrid parametric/stochastic programming [2, 26], (ii) process planning under uncertainty [39], (iii) scheduling under uncertainty [44], (iv) material design under uncertainty [15], (v) multi-objective optimization [33, 34, 42], (vi) flexibility analysis [7, 9], (vii) computation of singular multivariate normal probabilities [8], and (ix) solution of special cases of (1) [30]. While sensitivity analysis, which characterizes the optimal solution in the neighborhood of perturbed θ, has been widely studied and is available as a tool in many commercial softwares, parametric programming algorithms and softwares which characterize the solution for all the values of θ are relatively new [1, 3, 13, 14, 16, 17, 19, 24, 31, 33, 35, 37, 38, 47, 53, 54]. One very important application of parametric programming is in the area of online control and optimization where the optimal control variables are obtained explicitly as a function of the state variables and therefore online control and optimization problem reduces to a simple function evaluation problem [10, 28, 29, 36, 40, 41, 45, 46, 48–52]. So far this approach has focused on linear systems with quadratic objective functions. A solution technique for (2) would provide a major step in the direction of obtaining explicit solution of nonlinear optimal control problems.

While the ideas presented in this work are quite general, for the sake of simplicity in presentation, the discussions and illustrations will be centered around the case when the only nonconvexities in (2) are due to the presence of bilinear terms.

REMARK 3. For the case when nonconvexities other than bilinear terms are also present, it will be assumed that it is possible to create convex underestimating and overestimating functions of f and g and that the resulting estimating functions are continuously differentiable. See [5] for estimators for various types of nonconvex terms.

The basic idea of the B&B algorithm proposed in this work is to obtain parametric upper and lower bounds on the solution of (2). If the difference between the upper and lower bounds is within a certain tolerance, ϵ_1, the algorithm converges, otherwise for some x_j the interval $[x_j^L, x_j^U]$ is partitioned and tighter parametric lower and upper bounds are obtained. Note that a similar idea and a rudimentary prototype algorithm which relies on fixing and perturbing θ and solving the corresponding underestimating and overestimating subproblems is presented in [20]. Also note that a special case where f is concave, g is linear and $S=1$ is discussed in [11]. In this work, the upper and lower bounds are obtained by formulating and solving multiparametric convex overestimating and underestimating subproblems. The overestimating and underestimating subproblems are formulated by replacing the nonconvex terms in f and g by their convex underestimators and overestimators respectively. The resulting multiparametric convex problems are solved by using the procedure described in [16] a brief outline of which is presented in the next section. First note the following remark.

REMARK 4. Tighter overestimators of f and g in (2) and hence the tighter upper bounds on $z(\theta)$ would result in faster convergence of the solution procedure described in the last paragraph.

1.1. MULTIPARAMETRIC CONVEX NONLINEAR PROGRAMS

To facilitate the following discussion let $\check{f}$ and $\check{g}$ denote the convex underestimators of f and g respectively. For simplicity in presentation, assume that any additional variables that are required for defining $\check{g}$ are contained in x and therefore no new variables are defined. The aim is to solve the following multiparametric convex nonlinear programming problem:

$$\check{z}(\theta)=\min_{x}\check{f}(x) \tag{3.1}$$

$$\text{s.t.}\quad \check{g}_i(x)\leqslant b_i+F_i\theta,\quad i=1,\ldots,I \tag{3.2}$$

$$x_j^L\leqslant x_j\leqslant x_j^U,\, j=1,\ldots,J \tag{3.3}$$

$$x\in\Re^J \tag{3.4}$$

$$\theta\in\Theta\subseteq\Re^S. \tag{3.5}$$

Note that $\check{z}(\theta)$ is a convex and continuous function of θ [19]. An outer- approximation of (3) is obtained by formulating and solving the following multiparametric linear program:

$$\check{\check{z}}(\theta)=\min_{x}\check{f}(x^*)+\nabla_x\check{f}(x^*)(x-x^*) \tag{4.1}$$

$$\text{s.t.}\quad \check{g}(x^*)+\nabla_x\check{g}(x^*)(x-x^*)\leqslant b_i+F_i\theta,\quad i=1,\ldots,I \tag{4.2}$$

$$x_j^L\leqslant x_j\leqslant x_j^U\quad j=1,\ldots,J \tag{4.3}$$

$$x\in\Re^J \tag{4.4}$$

$$\theta\in\Theta\subseteq\Re^S, \tag{4.5}$$

where θ^* is an initial feasible point and x^* is the optimal solution of (3) for $\theta=\theta^*$. Note that the solution of (4) is given by a set of optimal solution profiles, $\check{\check{z}}(\theta)$, which are affine in θ and the corresponding polyhedral regions of optimality in Θ known as critical regions, CR, [24, 13]. Also note that $\check{\check{z}}(\theta)$ is a piecewise linear, continuous and convex function of θ [24]. Note that for convenience and simplicity in presentation, the notation CR is used to denote the set of points in the space of θ that lie in a CR as well as to denote the set of inequalities which define the CR. For a given CR the maximum difference between $\check{z}(\theta)$ and $\check{\check{z}}(\theta)$ will lie at one of the vertices of CR. At this vertex, θ^*, another mp-LP of the form (4) is formulated and solved to obtain another set of $\check{\check{z}}(\theta)$. This procedure of identifying θ^* and obtaining $\check{\check{z}}(\theta)$ continues until the maximum difference between $\check{z}(\theta)$ and $\check{\check{z}}(\theta)$ is within a pre-specified tolerance, ϵ_2. The tolerance ϵ_2 is then added to $\check{\check{z}}(\theta)$ to obtain $\check{z}(\theta)$. The final solution of (3) is given by linear parametric profiles and the corresponding regions of optimality. With this background it is now appropriate to start looking into the issues related to the solution of multiparametric nonconvex programs of the form (2). This is achieved by providing four motivating numerical examples in section 2.1 where issues that arise in obtaining parametric overestimators are discussed and in particular four different ways of obtaining parametric overestimators are presented. In section 2.2 an algorithm for solving (2) is presented and section 3 extends this for the case when 0–1 integer variables are also involved in (2). Two illustrative examples are presented in section 4, while concluding remarks are given in Section 5.

2. Multiparametric Non-Convex Nonlinear Programming

2.1. MOTIVATING EXAMPLES

EXAMPLE 1. Consider the following example:

$$z(\theta)=\min_x \cos(x) \tag{5.1}$$

$$\text{s.t.}\quad x\leqslant\theta \tag{5.2}$$

$$x\geqslant\theta \tag{5.3}$$

$$\pi\leqslant\theta\leqslant 5\pi, \tag{5.4}$$

where x and θ are scalars. The exact solution of this problem which is given by $z(\theta)=\cos(\theta)$ is plotted in Figure 1. Recall that in remark 1 it was noted that a local optimizer could be used to solve (1) to obtain an upper bound. In Section 1.1 a procedure was described which obtains the optimal solution for convex problems and hence could be thought of as a local parametric optimizer for solving (2). Next it is demonstrated that this procedure does not provide an upper bound on the solution of (2).

Let $\theta^*=\pi$ be a starting feasible point. An outer-approximation of (5) is given as follows:

$$z^{\mathrm{LOCAL}}(\theta)=\min_x -1 \tag{6.1}$$

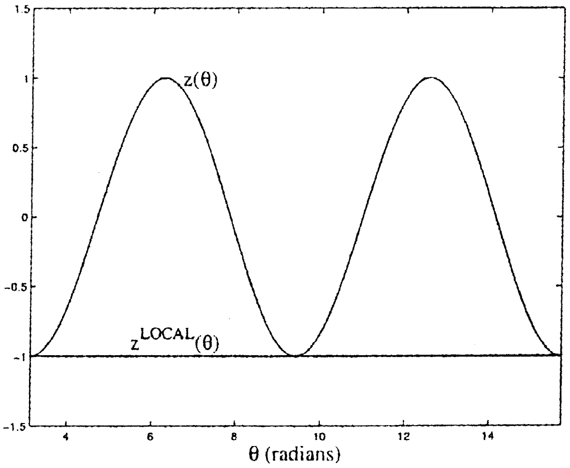

Figure 1. Example 1.

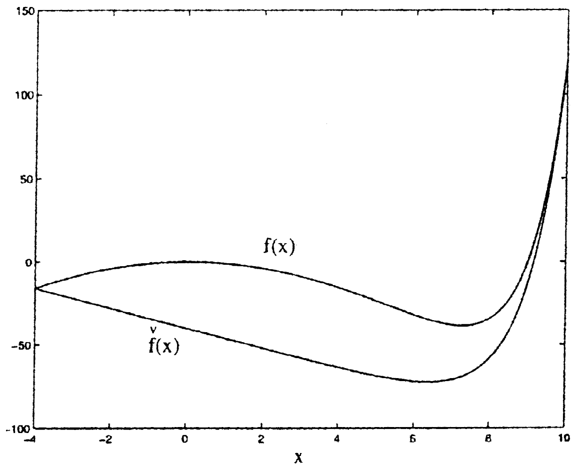

Figure 2. $f(x)$ and $\check{f}(x)$ for Example 2.

$$\text{s.t.}\quad x \leqslant \theta \tag{6.2}$$

$$x \geqslant \theta \tag{6.3}$$

$$\pi \leqslant \theta \leqslant 5\pi, \tag{6.4}$$

and its solution is given by $z^{\mathrm{LOCAL}}(\theta) = -1$ and the corresponding CR is given by $\pi \leqslant \theta \leqslant 5\pi$. The maximum difference between $z(\theta)$ and $z^{\mathrm{LOCAL}}(\theta)$ at the vertices of the CR is zero and hence the local parametric optimization procedure terminates. From Figure 1 note that $z^{\mathrm{LOCAL}}(\theta)$ is not an upper bound on $z(\theta)$.

REMARK 5. In general solving (2) by using the local parametric optimizer does not provide a parametric upper bound.

REMARK 6. A local solution of (1) at least provides a feasible solution. Even this property does not hold true for the case of (2). For example, if $z(\theta)$ is discontinuous then the solution obtained by the local parametric optimizer, which spans the complete range of θ simply by checking the solution at the vertices of the CR, may miss some discontinuities in between.

The next example demonstrates a way of obtaining parametric upper bound. This is followed by two examples which discuss four different ways of obtaining parametric upper bounds along with the relative merits in terms of computational requirements associated with obtaining each of the overestimators.

EXAMPLE 2. Consider the following example:

$$z(\theta)=\min_x f(x)=-x^2+0.01\exp(x) \tag{7.1}$$

$$\text{s.t.}\quad x\leqslant\theta \tag{7.2}$$

$$-4\leqslant x\leqslant 10 \tag{7.3}$$

$$-4\leqslant\theta\leqslant 10, \tag{7.4}$$

where x and θ are scalars. An underestimating subproblem of the form (3) for this example is given by:

$$\check{z}(\theta)=\min_x \check{f}(x)=-6x+0.01\exp(x)-40 \tag{8.1}$$

$$\text{s.t.}\quad x\leqslant\theta \tag{8.2}$$

$$-4\leqslant x\leqslant 10 \tag{8.3}$$

$$-4\leqslant\theta\leqslant 10. \tag{8.4}$$

Note that the underestimating subproblem (8) is obtained by replacing $-x^2$, the only nonconvex term in (7), by its linear convex underestimator. See Figure 2 where a plot of $f(x)$ and $\check{f}(x)$ is given. By using Figure 2, the solution of (8) is given by $x(\theta)=\theta$, $\forall\theta\in[-4,6.4]$ and $x(\theta)=6.4\forall\theta\in[6.4,10]$. This solution is inferred from Figure 2 by observing that $\check{f}(x)$ monotonically decreases as x increases from -4 to 6.4 and then $\check{f}(x)$ monotonically increases as x increases from 6.4 to 10 and by also keeping in mind the constraints on x and θ. Substituting this solution in $\check{f}(x)$ one obtains a parametric underestimator, $\check{z}^1(\theta)$, for (7) and since the constraints in (7) are convex, substitution of this solution in $f(x)$ provides an parametric overestimator or upper bound, $\hat{z}^1(\theta)$ – the superscript 1 denotes that these are obtained in the first iteration. Note that if the constraints were not convex then the solution must also be substituted into the constraints to check for feasibility. Also note that [11] suggested the substitution of the solution of the underestimating subproblem into $f(x)$ to obtain an upper bound for the case when f is concave, g is linear and θ is a scalar. See Figure 3 where $\check{z}^1(\theta)$ and $\hat{z}^1(\theta)$ are plotted. In the next step, $\check{z}^1(\theta)$ is compared to $\hat{z}^1(\theta)$ and the intervals of θ where $\hat{z}^1(\theta)-\check{z}^1(\theta)\leqslant\epsilon_1$, where ϵ_1 is a small positive tolerance, are fathomed. For this example $\epsilon_1=0$. From Figure 3 only $\theta=-4$ is fathomed and the next step is taken where the interval of x is divided into two smaller intervals: $[-4,0]$ and [0, 10] and the corresponding underestimating subproblems are formulated:

$$\check{z}^{2,1}(\theta)=\min_x \check{f}^{2,1}(x)=4x+0.01\exp(x) \tag{9.1}$$

$$\text{s.t.}\quad x\leqslant\theta \tag{9.2}$$

$$-4\leqslant x\leqslant 0 \tag{9.3}$$

$$-4\leqslant\theta\leqslant 10, \tag{9.4}$$

$$\check{z}^{2,2}(\theta)=\min_x \check{f}^{2,2}(x)=-10x+0.01\exp(x) \tag{10.1}$$

$$\text{s.t.}\quad x\leqslant\theta \tag{10.2}$$

$$0\leqslant x\leqslant 10 \tag{10.3}$$

$$-4\leqslant\theta\leqslant 10. \tag{10.4}$$

See Figure 4 where $\check{f}^{2,1}(x)$ and $\check{f}^{2,2}(x)$ for the corresponding intervals of validity are plotted. From Figure 4 the solution of (9) is given by: $x(\theta)=-4$, $\forall\theta\in[-4,10]$ and that of (10) is given by: $x(\theta)=\theta$, $\forall\theta\in[0,6.908]$ and $x(\theta)=6.908$, $\forall\theta\in[6.908,10]$. The corresponding $\check{z}^{2,1}(\theta)$ and $\check{z}^{2,2}(\theta)$ are plotted in Figure 5. Substitution of these solutions into $f(x)$ in (7) provides parametric overestimators or upper bounds, $\hat{z}^{2,1}(\theta)$ and $\hat{z}^{2,2}(\theta)$ which are plotted in Figure 6. Now all the three upper bounds, $\hat{z}^1(\theta)$, $\hat{z}^{2,1}(\theta)$ and $\hat{z}^{2,2}(\theta)$, that have been obtained so far are compared and a minimum of them over θ is obtained to give the current upper bound, $\bar{z}(\theta)$. Each of the lower bounds, $\check{z}^{2,1}(\theta)$ and $\check{z}^{2,2}(\theta)$ is then compared to $\bar{z}(\theta)$ – see Figure 7. $\check{z}^{2,1}(\theta)$ is within ϵ_1 of $\bar{z}(\theta)$ for all θ and therefore the interval $x\in[-4,0]$ is fathomed for all $\theta\in[-4,10]$. $\check{z}^{2,2}(\theta)$ is within ϵ_1 of $\bar{z}(\theta)$ for $\theta\in[-4,1.605]$ and therefore the interval $x\in[0,10]$ needs to be further branched. Just to recollect the results so far: $\bar{z}(\theta)$ is the final solution for $\theta\in[-4,1.605]$ and for $\theta\in[1.605,10]$ the interval of x that needs to be further explored is given by [0, 10]. Note the following remarks.

REMARK 7. For the solution of (2), parametric profiles and not simple numerical values need to be compared to make decisions regarding the fathoming step in the B&B tree.

REMARK 8. For the solution of (2), substitution of the solution of the underestimating subproblem into the original nonconvex problem results in an overestimator which in general may be nonlinear and nonconvex. For example see Figure 6.

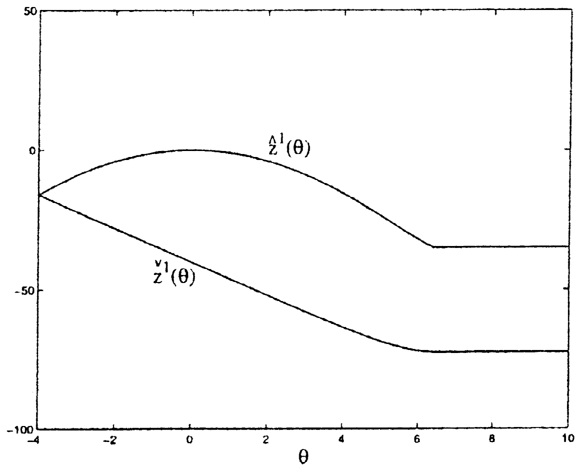

Figure 3. $\hat{z}^1(\theta)$ and $\check{z}^1(\theta)$ for Example 2.

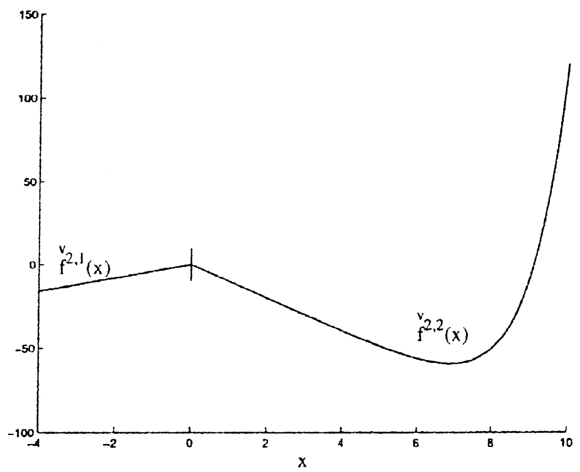

Figure 4. $\check{f}^{2,1}(x)$ and $\check{f}^{2,2}(x)$ for Example 2.

REMARK 9. For the case when $S=1$ comparison of nonlinear parametric profiles requires solution of a nonlinear equation per comparison. Intervals of θ where the solution has been found and where it has not been found are identified.

REMARK 10. For the case when $S\geqslant 2$ this comparison is much harder to perform and so is identifying the regions of θ where the solution has or has not been found. See Figure 8 for $S=2$ where a hypothetical case is shown and it is nontrivial to identify the regions in the space of θ where the linear parametric underestimator is within ϵ_1 of the nonlinear parametric upper bound. In general these regions would be nonlinear and nonconvex. Some initial thoughts on comparing nonlinear profiles were presented by [31].

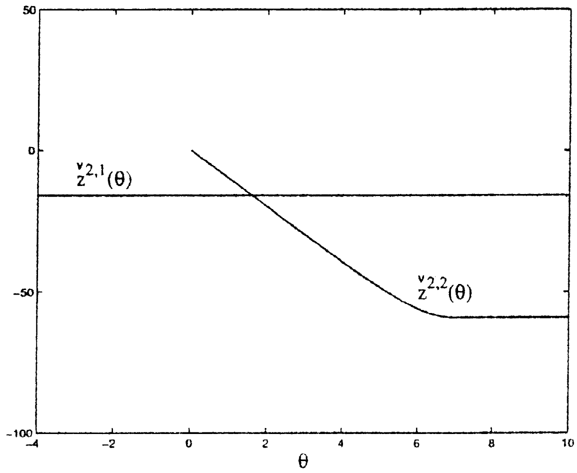

Figure 5. $\check{z}^{2,1}(\theta)$ and $\check{z}^{2,2}(\theta)$ for Example 2.

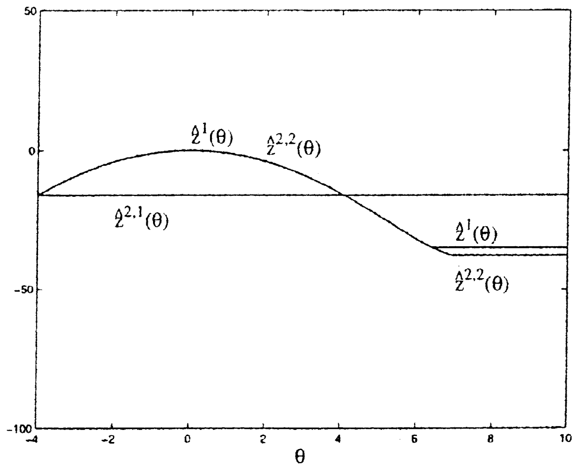

Figure 6. $\hat{z}^1(\theta)$, $\hat{z}^{2,1}(\theta)$ and $\hat{z}^{2,2}(\theta)$ for Example 2.

EXAMPLE 3. Consider an example with a bilinear objective and linear constraints:

$$z(\theta) = \min_x f(x) = x_1 x_2 \tag{11.1}$$

$$\text{s.t.}\quad 2x_1 + x_2 \geqslant \theta \tag{11.2}$$

$$x_1 + 3x_2 \geqslant 0.5\theta \tag{11.3}$$

$$-1 \leqslant x_1 \leqslant 1 \tag{11.4}$$

$$-1 \leqslant x_2 \leqslant 1 \tag{11.5}$$

$$0 \leqslant \theta \leqslant 1, \tag{11.6}$$

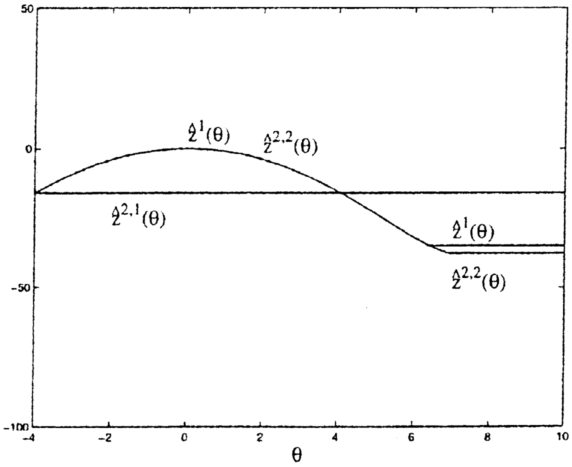

Figure 7. $\bar{z}(\theta)$, $\breve{z}^{2,1}(\theta)$ and $\breve{z}^{2,2}(\theta)$ for Example 2.

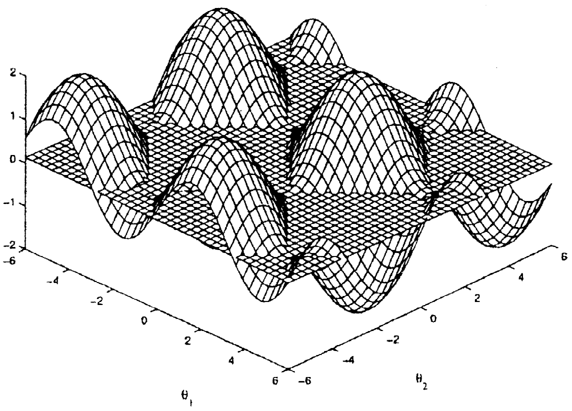

Figure 8. $\bar{z}(\theta)$ and $\breve{z}(\theta)$ for $S=2$.

where θ is a scalar. An underestimator of x_1x_2 can be obtained by replacing it by an additional variable $\breve{w}$ and introducing the following linear constraints [32]:

$$\breve{w} \geqslant x_1^L x_2 + x_2^L x_1 - x_1^L x_2^L \tag{12.1}$$

$$\breve{w} \geqslant x_1^U x_2 + x_2^U x_1 - x_1^U x_2^U. \tag{12.2}$$

Similar overestimating linear constraints are given as follows:

$$\hat{w} \leqslant x_1^L x_2 + x_2^U x_1 - x_1^L x_2^U \tag{13.1}$$

$$\hat{w} \geqslant x_1^U x_2 + x_2^L x_1 - x_1^U x_2^L. \tag{13.2}$$

The underestimating subproblem of (11) is formulated by using (12) as follows:

$$\check{z}(\theta)=\min_{x,\check{w}} \check{w} \tag{14.1}$$

$$\text{s.t.}\quad \check{w} \geqslant -x_2-x_1-1 \tag{14.2}$$

$$\check{w} \geqslant x_2+x_1-1 \tag{14.3}$$

$$2x_1+x_2 \geqslant \theta \tag{14.4}$$

$$x_1+3x_2 \geqslant 0.5\theta \tag{14.5}$$

$$-1 \leqslant x_1 \leqslant 1 \tag{14.6}$$

$$-1 \leqslant x_2 \leqslant 1 \tag{14.7}$$

$$0 \leqslant \theta \leqslant 1. \tag{14.8}$$

The solution of (14) is given by: $\check{w}=0.5\theta-1$, $x_1=0.5\theta$, $x_2=0$, $\check{z}(\theta)=0.5\theta-1$, $\forall\theta\in[0,1]$. Now overestimators of $z(\theta)$ can be created in the following four ways.

OVERESTIMATOR-1, $\hat{z}_{O1}(\theta)$: Substitution of the solution of (14) into $f(x)$ in (11) gives the following overestimator: $\hat{z}_{O1}(\theta)=0$.

OVERESTIMATOR-2, $\hat{z}_{O2}(\theta)$: Another overestimator can be created based upon the following lemma.

LEMMA 1. [6] *The maximum separation between x_1x_2 and $\check{w}$ inside the rectangle $[x_1^L,x_1^U]\times[x_2^L,x_2^U]$ is equal to $\delta_{12}=(x_1^U-x_1^L)(x_2^U-x_2^L)/4$.*

LEMMA 2. *If $f(x)=f^c(x)+\sum_{j=1}^J\sum_{j'=1}^J a_{jj'}x_jx_{j'}$, where $j\neq j'$, $f^c(x)$ is a convex function of x, $a_{jj'}$ is constant and positive for all j and j' (without loss of generality, we assume $a_{jj'}>0$; for some $a_{jj'}<0$ the following results can be accordingly modified) and g is convex then $\hat{z}_{O2}(\theta)=\check{z}(\theta)+\sum_{j=1}^J\sum_{j'=1}^J a_{jj'}\delta_{jj'}$ where $\delta_{jj'}=(x_j^U-x_j^L)(x_{j'}^U-x_{j'}^L)/4$. Note that terms of the form $a_{jj'}x_jx_{j'}$, $j=j'$ are convex and a part of the convex function $f^c(x)$.*

Proof. Consider the following problem:

$$z(\theta)=\min_x f^c(x)+\sum_{j=1}^J\sum_{j'=1}^J a_{jj'}x_jx_{j'} \tag{15.1}$$

$$\text{s.t.}\quad g_i(x)\leqslant b_i+F_i\theta,\quad i=1,\dots,I \tag{15.2}$$

$$x_j^L\leqslant x_j\leqslant x_j^U,\quad j=1,\dots,J \tag{15.3}$$

$$x\in\Re^J \tag{15.4}$$

$$\theta\in\Theta\subseteq\Re^S, \tag{15.5}$$

where $j \neq j'$ and $a_{jj'}$ is constant and positive for all j and j'. A convex underestimating subproblem of (15) by using (12) is given as follows:

$$\check{z}(\theta) = \min_{x,\check{w}} f^c(x) + \sum_{j=1}^{J}\sum_{j'=1}^{J} a_{jj'}, \check{w}_{jj'} \tag{16.1}$$

$$\text{s.t.} \quad g_i(x) \leqslant b_1 + F_i\theta, i = 1, \ldots, I \tag{16.2}$$

$$\check{w}_{jj'} \geqslant x_j^L x_{j'} + x_{j'}^L x_j - x_j^L x_{j'}^L, \quad j, j' = 1, \ldots, J \tag{16.3}$$

$$\check{w}_{jj'} \geqslant x_j^U x_{j'} + x_{j'}^U x_j - x_j^U x_{j'}^U, \quad j, j' = 1, \ldots, J \tag{16.4}$$

$$x_j^L \leqslant x_j \leqslant x_j^U, \quad j = 1, \ldots, J \tag{16.5}$$

$$x \in \Re^J \tag{16.6}$$

$$\theta \in \Theta \subseteq \Re^S. \tag{16.7}$$

By using Lemma 1 an overestimating subproblem of (15) can be constructed from (16) as follows:

$$\hat{z}_{O2}(\theta) = \min_{x,\hat{w}} f^c(x) + \sum_{j=1}^{J}\sum_{j'=1}^{J} a_{jj'}, \hat{w}_{jj'} \tag{17.1}$$

$$\text{s.t.} \quad g_i(x) \leqslant b_i + F_i\theta, i = 1, \ldots, I \tag{17.2}$$

$$\hat{w}_{jj'} \geqslant x_j^L x_{j'} + x_{j'}^L x_j - x_j^L x_{j'}^L + \delta_{jj'}, \quad j, j' = 1, \ldots, J \tag{17.3}$$

$$\hat{w}_{jj'} \geqslant x_j^U x_{j'} + x_{j'}^U x_j - x_j^U x_{j'}^U + \delta_{jj'}, \quad j, j' = 1, \ldots, J \tag{17.4}$$

$$x_j^L \leqslant x_j \leqslant x_j^U, \quad j = 1, \ldots, J \tag{17.5}$$

$$x \in \Re^J \tag{17.6}$$

$$\theta \in \Theta \subseteq \Re^S. \tag{17.7}$$

where $\delta_{jj'} = (x_j^U - x_j^L)(x_{j'}^U - x_{j'}^L)/4$. By defining $\bar{w}_{jj'} = \hat{w} - \delta_{jj'}$, $\forall j, j' = 1, \ldots, J$, $j \neq j'$, (17) can be formulated as follows:

$$\hat{z}_{O2}(\theta) = \min_{x,\bar{w}} f^c(x) + \sum_{j=1}^{J}\sum_{j'=1}^{J} a_{jj'}, \bar{w}_{jj'} + \sum_{j=1}^{J}\sum_{j'=1}^{J} a_{jj'}, \delta_{jj'} \tag{18.1}$$

$$\text{s.t.} \quad g_i(x) \leqslant b_i + F_i\theta, i = 1, \ldots, I \tag{18.2}$$

$$\bar{w}_{jj'} \geqslant x_j^L x_{j'} + x_{j'}^L x_j - x_j^L x_{j'}^L, \quad j, j' = 1, \ldots, J \tag{18.3}$$

$$\bar{w}_{jj'} \geqslant x_j^U x_{j'} + x_{j'}^U x_j - x_j^U x_{j'}^U, \quad j, j' = 1, \ldots, J \tag{18.4}$$

$$x_j^L \leqslant x_j \leqslant x_j^U, \quad j = 1, \ldots, J \tag{18.5}$$

$$x \in \Re^J \tag{18.6}$$

$$\theta \in \Theta \subseteq \Re^S. \tag{18.7}$$

By comparing (16) and (18), $\hat{z}_{O2}(\theta)=\check{z}(\theta)+\sum_{j=1}^{J}\sum_{j'=1}^{J}a_{jj'}\delta_{jj'}$.

Therefore for the current example $\hat{z}_{O2}(\theta)=\check{z}(\theta)+\delta_{12}=0.5\theta$.

OVERESTIMATOR-3, $\hat{z}_{O3}(\theta)$: While the first two overestimators were obtained with negligible effort after the underestimating subproblem had been solved the remaining two overestimators require formulating and solving overestimating subproblems. First overestimating subproblem is formulated as follows:

$$\hat{z}_{O3}(\theta)=\min_{x,\hat{w}}\hat{w} \tag{19.1}$$

$$\text{s.t.}\quad \hat{w}\geqslant -x_2+x_1+1 \tag{19.2}$$

$$\hat{w}\geqslant x_2-x_1+1 \tag{19.3}$$

$$2x_1+x_2\geqslant\theta \tag{19.4}$$

$$x_1+3x_2\geqslant 0.5\theta \tag{19.5}$$

$$-1\leqslant x_1\leqslant 1 \tag{19.6}$$

$$-1\leqslant x_2\leqslant 1 \tag{19.7}$$

$$0\leqslant\theta\leqslant 1. \tag{19.8}$$

Note that the McCormick overestimators (13) are used except that the sign of the less than inequalities has been changed to the greater than inequalities as follows:

$$\hat{w}\geqslant x_1^L x_2+x_2^U x_1-x_1^L x_2^U \tag{20.1}$$

$$\hat{w}\geqslant x_1^U x_2+x_2^L x_1-x_1^U x_2^L. \tag{20.2}$$

The solution of (19) is given by $\hat{z}_{O3}(\theta)=1$.

OVERESTIMATOR-4, $\hat{z}_{O4}(\theta)$: Another overestimating subproblem can be formulated as follows:

$$\hat{z}_{O4}(\theta)=\max_{x,\hat{w}}\hat{w} \tag{21.1}$$

$$\text{s.t.}\quad \hat{w}\leqslant -x_2+x_1+1 \tag{21.2}$$

$$\hat{w}\leqslant x_2-x_1+1 \tag{21.3}$$

$$2x_1+x_2\geqslant\theta \tag{21.4}$$

$$x_1+3x_2\geqslant 0.5\theta \tag{21.5}$$

$$-1\leqslant x_1\leqslant 1 \tag{21.6}$$

$$-1\leqslant x_2\leqslant 1 \tag{21.7}$$

$$0\leqslant\theta\leqslant 1. \tag{21.8}$$

The things to be noted are that the less than inequalities in (13) have been retained and the problem now is formulated as to maximize and not minimize $\hat{w}$. The solution is given by $\hat{z}_{O4}(\theta)=1$. Also note that it is not always possible to obtain $\hat{z}_{O4}(\theta)$ as illustrated next. Consider a modification of (11) where $f(x) = x_1x_2 + 100x_1 + 100x_2$. An underestimator for the modified problem is given by $\check{z}(\theta) = 50.5\theta - 1$, $\forall\theta \in [0,1]$. An attempt to maximize $\hat{f}(x) = \hat{w} - 100x_1 - 100x_2$ subject to the constraints in (21.2)–(21.8) gives $\hat{z}(\theta) = -50.5\theta + 1$, which is not a valid overestimator. One obvious thought that comes to mind is that why maximize $\hat{f}(x) = \hat{w} - 100x_1 - 100x_2$ and not $\hat{f}(x) = \hat{w} + 100x_1 + 100x_2$. The reasons for this are that (i) the terms $100x_1 + 100x_2$ in $f(x)$, the original objective function, were supposed to be minimized and not maximized and (ii) if, for example, the terms $100x_1{}^2 + 100x_2{}^2$ were present instead of $100x_1 + 100x_2$ then maximization of $\hat{f}(x) = \hat{w} + 100x_1{}^2 + 100x_2{}^2$ is a nonconvex optimization problem, while the objective was to obtain a convex overestimator.

REMARK 11. It is not always possible to obtain $\hat{z}_{O4}(\theta)$ if convex terms are also present in addition to bilinear terms in $f(x)$. If only bilinear terms are present in the objective function then $\hat{z}_{O4}(\theta) \leqslant \hat{z}_{O3}(\theta)$. This can be interpreted by plotting the right hand sides of (13) as a function of x_1 and x_2 for some fixed values of x_1^L, x_1^U, x_2^L, and x_2^U.

EXAMPLE 4. Consider an example with a bilinear term in the constraints:

$$z(\theta) = \min_x f(x) = x_1 + x_2 \tag{22.1}$$
$$\text{s.t.}\quad 2x_1 + x_2 \geqslant \theta \tag{22.2}$$
$$x_1 + 3x_2 \geqslant 0.5\theta \tag{22.3}$$
$$4x_1 + x_2 + x_1x_2 \leqslant 0.25\theta \tag{22.4}$$
$$-1 \leqslant x_1 \leqslant 1 \tag{22.5}$$
$$-1 \leqslant x_2 \leqslant 1 \tag{22.6}$$
$$0 \leqslant \theta \leqslant 1. \tag{22.7}$$

The understanding subproblem is given as follows:

$$\check{z}(\theta) = \min_{x,\check{w}} f(x) = x_1 + x_2 \tag{23.1}$$
$$\text{s.t.}\quad 2x_1 + x_2 \geqslant \theta \tag{23.2}$$
$$x_1 + 3x_2 \geqslant 0.5\theta \tag{23.3}$$
$$4x_1 + x_2 + \check{w} \leqslant 0.25\theta \tag{23.4}$$
$$\check{w} \geqslant -x_2 - x_1 - 1 \tag{23.5}$$
$$\check{w} \geqslant x_2 + x_1 - 1 \tag{23.6}$$
$$-1 \leqslant x_1 \leqslant 1 \tag{23.7}$$
$$-1 \leqslant x_2 \leqslant 1 \tag{23.8}$$
$$0 \leqslant \theta \leqslant 1. \tag{23.9}$$

The solution of (23) is given by: $x_1 = 0.5\theta$, $x_2 = 0$, $\check{w} = 0.5\theta - 1$, $\check{z}(\theta) = 0.5\theta$, $\forall\theta \in [0, 0.444]$ and $x_1 = -1.75\theta + 1$, $x_2 = 4.5\theta - 2$, $\check{w} = 2.75\theta - 2$, $\check{z}(\theta) =$

$2.75\theta-1, \forall\theta\in[0.444, 0.6667]$. The problem is infeasible $\forall\theta\in[0.6667, 1]$ and therefore $\check{z}(\theta)=\infty, \forall\theta\in[0.6667, 1]$. The overestimators are obtained as follows.

OVERESTIMATOR-1, $\hat{z}_{O1}(\theta)$: Substitution of the solution of (23) into $f(x)$ and in (22.4) gives the following overestimator: $\hat{z}_{O1}(\theta)=0.5\theta$, $\forall\theta\in[0]$ and $\hat{z}_{O1}(\theta)=2.75\theta-1$, $\forall\theta\in[0.444, 0.6667]$. Note that for this example the solution of the underestimating subproblem is substituted into the objective function as well as constraints since one of the constraints is nonconvex.

OVERESTIMATOR-2, $\hat{z}_{O2}(\theta)$: an overestimating subproblem for (22) can be formulated by using Lemma 1 as follows:

$$\hat{z}_{O2}(\theta)=\min_{x,\hat{w}} f(x)=x_1+x_2 \tag{24.1}$$

$$\text{s.t.}\quad 2x_1+x_2\geqslant\theta \tag{24.2}$$

$$x_1+3x_2\geqslant 0.5\theta \tag{24.3}$$

$$4x_1+x_2+\hat{w}\leqslant 0.25\theta \tag{24.4}$$

$$\hat{w}\geqslant -x_2-x_1 \tag{24.5}$$

$$\hat{w}\geqslant x_2+x_1 \tag{24.6}$$

$$-1\leqslant x_1\leqslant 1 \tag{24.7}$$

$$-1\leqslant x_2\leqslant 1 \tag{24.8}$$

$$0\leqslant\theta\leqslant 1. \tag{24.9}$$

Note that the overestimators in (24) for the bilinear term in (22) are obtained by using the McCormick underestimators in (12) and adding δ_{12} from Lemma 1 as follows:

$$\hat{w}\geqslant x_1^L x_2+x_2^L x_1-x_1^L x_2^L+\delta_{12} \tag{25.1}$$

$$\hat{w}\geqslant x_1^U x_2+x_2^U x_1-x_1^U x_2^U+\delta_{12}. \tag{25.2}$$

The solution of (24) is given by: $\hat{z}_{O2}(\theta)=2.75\theta$, $\forall\theta\in[0, 0.22]$.

REMARK 12. In some cases $\hat{z}_{O2}(\theta)$ can be obtained more efficiently – by avoiding solving a parametric optimization problem of the form (24) and solving only the underestimating subproblem of the form (23) – although for an interval of θ that is bigger than given in the original problem. For example, consider the following problem:

$$z(\theta)=\min_{x} f^c(x) \tag{26.1}$$

$$\text{s.t.}\quad g_i^c(x)\leqslant b_i, i=1,\ldots,I, i\neq i' \tag{26.2}$$

$$g_{i'}^c(x)+x_1x_2\leqslant F_{i'1}\theta \tag{26.3}$$

$$x_j^L \leqslant x_j \leqslant x_j^U, \quad j=1,\ldots,J \tag{26.4}$$

$$x \in \Re^J \tag{26.5}$$

$$\theta^L \leqslant \theta \leqslant \theta^U \tag{26.6}$$

where $f^c(x), g_i^c(x)$ and $g_{i'}^c(x)$ are convex functions of x and θ is a scalar bounded between θ^L and θ^U. An underestimating subproblem for (26) is given by:

$$\check{z}(\theta) = \min_{x,\check{w}} f^c(x) \tag{27.1}$$

$$\text{s.t.} \quad g_i^c(x) \leqslant b_i, \; i=1,\ldots,I, i \neq i' \tag{27.2}$$

$$g_{i'}^c(x) + \check{w} \leqslant F_{i'1}\theta \tag{27.3}$$

$$\check{w} \geqslant x_1^L x_2 + x_2^L x_1 - x_1^L x_2^L \tag{27.4}$$

$$\check{w} \geqslant x_1^U x_2 + x_2^U x_1 - x_1^U x_2^U \tag{27.5}$$

$$x_j^L \leqslant x_j \leqslant x_j^U, \; j=1,\ldots,J \tag{27.6}$$

$$x \in \Re^J \tag{27.7}$$

$$\theta^L \leqslant \theta \leqslant \theta^U. \tag{27.8}$$

Similarly an overestimating subproblem is given by:

$$\hat{z}_{O2}(\theta) = \min_{x,\hat{w}} f^c(x) \tag{28.1}$$

$$\text{s.t.} \quad g_i^c(x) \leqslant b_i, \; i=1,\ldots,I, i \neq i' \tag{28.2}$$

$$g_{i'}^c(x) + \hat{w} \leqslant F_{i'1}\theta \tag{28.3}$$

$$\hat{w} \geqslant x_1^L x_2 + x_2^L x_1 - x_1^L x_2^L + \delta_{12} \tag{28.4}$$

$$\hat{w} \geqslant x_1^U x_2 + x_2^U x_1 - x_1^U x_2^U + \delta_{12} \tag{28.5}$$

$$x_j^L \leqslant x_j \leqslant x_j^U, \; j=1,\ldots,J \tag{28.6}$$

$$x \in \Re^J \tag{28.7}$$

$$\theta^L \leqslant \theta \leqslant \theta^U. \tag{28.8}$$

Subtracting δ_{12} from (28.3)–(28.5) and defining $\bar{w} = \hat{w} - \delta_{12}$, (28) can be formulated as:

$$\hat{z}_{O2}(\theta) = \min_{x,\bar{w}} f^c(x) \tag{29.1}$$

$$\text{s.t.} \quad g_i^c(x) \leqslant b_i, \; i=1,\ldots,I, i \neq i' \tag{29.2}$$

$$g_{i'}^c(x) + \bar{w} \leqslant F_{i'1}\theta - \delta_{12} \tag{29.3}$$

$$\bar{w} \geqslant x_1^L x_2 + x_2^L x_1 - x_1^L x_2^L \tag{29.4}$$

$$\bar{w} \geqslant x_1^U x_2 + x_2^U x_1 - x_1^U x_2^U \quad (29.5)$$

$$x_j^L \leqslant x_j \leqslant x_j^U, \; j=1,\dots,J \quad (29.6)$$

$$x \in \Re^J \quad (29.7)$$

$$\theta^L \leqslant \theta \leqslant \theta^U. \quad (29.8)$$

Note that the only difference between (27) and (29) is in (27.3) and (29.3), which essentially means that (29) is solved for a shifted interval of θ. This means that for $F_{i'1} > 0$, if (27) is solved for θ in the expanded interval $[\theta^L - \delta_{12}/F_{i'1}, \theta^U]$, then the solution of (29) can be inferred from the solution of (27). The corresponding expanded interval when $F_{i'1} < 0$ is given by $[\theta^L, \theta^U - \delta_{12}/F_{i'1}]$. Note that this option of solving (27) for an expanded interval of θ will be computationally attractive if the shift, $\delta_{12}/F_{i'1}$, does not significantly expand the original interval $[\theta^L, \theta^U]$, i.e., there is at least some overlap between the expanded and the original interval. This can be checked in a pre-processing step. The above mentioned procedure can be generalized for the case when θ is a vector and present in more than one constraint and also when there are some more nonconvex terms in (26). For generalization of the procedure one should be able to formulate one problem for which the solution space covers the solution space of both the underestimating and the overestimating subproblems.

OVERESTIMATOR-3, $\hat{z}_{O3}(\theta)$: Another way of obtaining an overestimator is to solve the following problem:

$$\hat{z}_{O3}(\theta) = \min_{x,\hat{w}} f(x) = x_1 + x_2 \quad (30.1)$$

$$\text{s.t.} \quad 2x_1 + x_2 \geqslant \theta \quad (30.2)$$

$$x_1 + 3x_2 \geqslant 0.5\theta \quad (30.3)$$

$$4x_1 + x_2 + \hat{w} \leqslant 0.25\theta \quad (30.4)$$

$$\hat{w} \geqslant -x_2 + x_1 + 1 \quad (30.5)$$

$$\hat{w} \geqslant x_2 - x_1 + 1 \quad (30.6)$$

$$-1 \leqslant x_1 \leqslant 1 \quad (30.7)$$

$$-1 \leqslant x_2 \leqslant 1 \quad (30.8)$$

$$0 \leqslant \theta \leqslant 1, \quad (30.9)$$

where the overestimators are obtained by using (20). (30) does not have a feasible solution and therefore $\hat{z}_{O3}(\theta) = \infty$.

LEMMA 3. *The overestimator in* (25), *which corresponds to* $\hat{z}_{O2}(\theta)$, *is tighter than the overestimator in* (20), *which corresponds to* $\hat{z}_{O3}(\theta)$, *in* 87.5% *of the area* *of the rectangle* $[x_1^L, x_1^U] \times [x_2^L, x_2^U]$ *provided that the rectangle is not empty. The proof is easy and not presented.*

REMARK 13. Note that so far we have focussed on the case where δ_{12} for bilinear terms was given [6]. For the case when general nonconvex terms are also involved then [6] showed that the maximum separation between a nonconvex term and its underestimator is bounded and proportional to a positive parameter and the square of the diagonal of the current box constraints on x. Expressions for the maximum separation distance for fractional terms have been presented in [4].

OVERESTIMATOR-4, $\hat{z}_{O4}(\theta)$: It is not possible to obtain $\hat{z}_{O4}(\theta)$ because the nonconvexity appears in the constraints and not in the objective function.

2.2. MULTIPARAMETRIC NONCONVEX PROGRAMMING: THEORY AND ALGORITHM

The central idea behind the solution of (2) is to create convex parametric underestimators and overestimators, denoted by $\check{z}(\theta)$ and $\hat{z}(\theta)$ respectively, of $z(\theta)$ and then branch and bound on x until the difference between $\hat{z}(\theta)$ and $\check{z}(\theta)$ is within a certain pre-specified tolerance, ϵ_1 (Remarks 4–7). The difference between $\hat{z}(\theta)$ and $\check{z}(\theta)$ will be referred to as "Global Parametric Gap". Note that for the case when $\hat{z}(\theta)$ and $\check{z}(\theta)$ are affine in θ the global parametric gap is checked by using a comparison procedure proposed by [3] which is summarized in Appendix A. The parametric underestimators are obtained by creating convex underestimators of f and g and then formulating and solving problem (3) as described in Section 1.1. The solution of (3) is given by linear parametric profiles and the corresponding critical regions. Convex parametric overestimators can also be similarly obtained by creating convex overestimators of f and g and solving the resulting multiparametric convex nonlinear program as described in Section 1.1. The final solution would again be given by linear parametric profiles and the corresponding critical regions. In some cases it is not required to formulate and solve an overestimating subproblem and instead a parametric overestimator can be obtained merely from the solution of the underestimating subproblem – these cases were discussed in Section 2.1. Four different ways of obtaining parametric overestimators were discussed and the key features of each of the parametric overestimators were also presented. The relative merits of different types of parametric overestimators can be weighed in terms of three attributes: (i) ease of obtaining, (ii) tightness and (iii) functional description, i.e., linear or nonlinear. These issues are briefly reviewed next.

Parametric overestimator of type-1, which is denoted by $\hat{z}(\theta)_{O1}$, is perhaps the easiest one to obtain because it requires the substitution of the solution of the underestimating subproblem, (3), into the original problem, (2). One disadvantage is that, in general, it may lead to nonlinear and nonconvex functional description of $\hat{z}(\theta)_{O1}$

and corresponding critical regions. In such cases comparison of $\hat{z}(\theta)_{O1}$ to $\check{z}(\theta)$ is nontrivial (Remarks 8–10). For the cases (i) when $S=1$, the comparison is easier (Remark 9) and (ii) when $\hat{z}(\theta)_{O1}$ simplifies to affine expressions in θ ($\hat{z}(\theta)_{O1}$ in Examples 3 and 4), the comparison is much simpler and can be achieved by the procedure of [3] described in Appendix A.

$\hat{z}(\theta)_{O2}$, the overestimator of the second type, which is based upon the work of Floudas and co-workers (Lemma 1), also has the advantage that it can be obtained with negligible effort after the underestimating subproblem has been solved (Lemma 2). This feature holds true for the case when the only nonconvex terms are bilinear terms and these terms are present only in the objective function. For the case when bilinear terms are also present in the constraints there are some cases where $\hat{z}(\theta)_{O2}$ can be obtained more effficiently at modest extra effort (Remark 12). Since the underestimator is affine in θ, $\hat{z}(\theta)_{O2}$ is also afffine in θ and the comparison can be carried out ([3], Appendix A). The extension of these ideas for the case when general nonconvex terms are present is also possible along the work of Floudas and co-workers (Remark 13).

Unlike for the case of $\hat{z}(\theta)_{O1}$ and many cases of $\hat{z}(\theta)_{O2}$, the overestimator of the third type, $\hat{z}(\theta)_{O3}$, requires solving a parametric optimization problem. The key advantage is that this type of formulation is completely general and does not have limitations regarding the presence of only bilinear terms and restrictions regarding nonconvex terms only in the objective function (Remark 3). For the case of bilinear terms the overestimating expressions, used for $\hat{z}(\theta)_{O3}$, are less tight than the ones used for $\hat{z}(\theta)_{O2}$in 87.5% of the area of the rectangle $[x_1^L, x_1^U]\times[x_2^L, x_2^U]$ (Lemma 3). The solution is affine in θ and can be compared to $\check{z}(\theta)$.

The fourth type of overestimator, $\hat{z}(\theta)_{O4}$, also requires solving a parametric optimization problem. It is tighter than $\hat{z}(\theta)_{O3}$ but is limited to the case when only bilinear terms are present in the objective function because it relies on maximization of the auxiliary variables, $\hat{w}$, which replace the bilinear terms (Remark 11 and $\hat{z}(\theta)_{O4}$ in Example 4).

Based upon the above developments an algorithm for the solution of (2) is presented in Table 1. It is assumed that the parametric overestimators can be compared to the parametric underestimators by using the comparison procedure ([3], Appendix A) – which is always the case in $\hat{z}(\theta)_{O2}$, $\hat{z}(\theta)_{O3}$ and $\hat{z}(\theta)_{O4}$ and sometimes is the case in $\hat{z}(\theta)_{O1}$.

For general nonconvex problems, it is not obvious which overestimator will perform better than the other one, as the performance is dependent upon problem types and particular examples under consideration. Some general remarks and lemmas regarding the (i) effort required to obtain these overestimators, (ii) tightness and (iii) effort required to compare to the underestimators have been presented. These are quite important issues which afffect the overall performance of the algorithm. In the next section, the case where 0–1 binary variables are also involved in (2) is considered.

Table 1. Multiparametric global optimization algorithm

Step 1. Initialize the current upper bound as $\bar{z}(\theta)=\infty$, a region of θ, CR, a space of continuous variables x – determined by the lower and upper bounds x^L and x^U respectively, and tolerances, ϵ_1 and ϵ_2.

Step 2. For a given region of θ, CR, and the corresponding space of x,
- (a) formulate and solve (3) as described in section 1.1 and obtain the parametric underestimators, $\check{z}(\theta)$.
- (b) obtain the parametric overestimators, $\hat{z}(\theta)$, by using one of the methods described in Sections 2.1 and 2.2.

Step 3. Compare $\hat{z}(\theta)$ to $\bar{z}(\theta)$, as described in Appendix A, and update the current upper bound $\bar{z}(\theta)=\min(\hat{z}(\theta),\bar{z}(\theta))$, in the corresponding regions of θ.

Step 4. Compare $\check{z}(\theta)$ to $\bar{z}(\theta)$, as described in Appendix A, and in the spaces of x where,
- (a) $\check{z}(\theta)\leqslant\bar{z}(\theta)-\epsilon_1$, branch on x by subdividing the bounds on x and go to Step 2,
- (b) $\check{z}(\theta)\geqslant\bar{z}(\theta)-\epsilon_2$, fathom those spaces of x only for the corresponding regions of θ.

Step 5. In the spaces of x where (3) is infeasible, fathom those spaces and the corresponding regions of θ.

Step 6. If no more spaces of x and regions of θ to explore, terminate, or otherwise go to Step 2.

Step 7. The final solution is given by $\bar{z}(\theta)$.

3. Multiparametric Mixed-Integer Nonconvex Programming

Consider the following multiparametric mixed-integer nonlinear programming problem:

$$z(\theta)=\min_{x,y} f(x,y) \tag{31.1}$$

$$\text{s.t.}\quad g_i(x,y)\leqslant b_i+F_i\theta,\; i=1,\ldots,I \tag{31.2}$$

$$x_j^L\leqslant x_j\leqslant x_j^U,\; j=1,\ldots,J \tag{31.3}$$

$$y\in\{0,1\}^M \tag{31.4}$$

$$x\in\Re^J \tag{31.5}$$

$$\theta\in\Theta\subseteq\Re^S, \tag{31.6}$$

where y is a vector of 0-1 binary variables. The basic idea of the algorithm for the solution of (31) is to obtain a parametric solution for y fixed at integer values and then use this solution as the current solution to cut-off suboptimal integer solutions and identify the ones that are better than the current one. The better integer solutions that are identified then become the current solution and this procedure continues until all the optimal solutions and the corresponding regions of optimality, in the space of θ, have been identified. An initial integer solution is identified by solving the following problem:

$$\min_{x,y,\theta} f(x,y) \tag{32.1}$$

$$\text{s.t.} \quad g_i(x,y) - F_i\theta \leqslant b_i, \ i=1,\dots,I \tag{32.2}$$

$$x_j^L \leqslant x_j \leqslant x_j^U, \ j=1,\dots,J \tag{32.3}$$

$$y \in \{0,1\}^M \tag{32.4}$$

$$x \in \Re^J \tag{32.5}$$

$$\theta \in \Theta \subseteq \Re^S, \tag{32.6}$$

where θ is treated as a vector of free variables. See [4] for an algorithm for the solution of (32). Let the solution of (32) be given by $y=\tilde{y}$. The algorithm starts by fixing $y=\tilde{y}$ in (31) to obtain the following nonconvex mp-NLP:

$$z_{\tilde{y}}(\theta) = \min_{x} f(x,\tilde{y}) \tag{33.1}$$

$$\text{s.t.} \quad g_i(x,\tilde{y}) \leqslant b_i + F_i\theta, \ i=1,\dots,I \tag{33.2}$$

$$x_j^L \leqslant x_j \leqslant x_j^U, \ j=1,\dots,J \tag{33.3}$$

$$x \in \Re^J \tag{33.4}$$

$$\theta \in \Theta \subseteq \Re^S. \tag{33.5}$$

The solution of (33) is then approached by creating convex underestimators and overestimators of nonconvex functions $f(x,\tilde{y})$ and $g(x,\tilde{y})$ which converge to the global optima by branching on the space of x – similar to solution of (2). The lth solution of (33), $z_{\tilde{y}}(\theta)^l$, which is given by a linear parametric profile valid in its region of optimality, CR^l represents a current upper bound in CR^l. Another optimal vector of integer variables is then obtained in each region CR^l by formulating the following problem:

$$\min_{x,y,\theta} f(x,y) \tag{34.1}$$

$$\text{s.t.} \quad g_i(x,y) \leqslant b_i + F_i\theta, \ i=1,\dots,I \tag{34.2}$$

$$f(x,y) \leqslant \hat{z}(\theta)^l \tag{34.3}$$

$$\sum_{n\in N^{lk}} y_n^{lk} - \sum_{n\in P^{lk}} y_n^{lk} \leqslant |N^{lk}| - 1, \ k=1,\dots,K^l \tag{34.4}$$

$$x_j^L \leqslant x_j \leqslant x_j^U, \ j=1,\dots,J \tag{34.5}$$

$$y \in \{0,1\}^M \tag{34.6}$$

$$x \in \Re^J \tag{34.7}$$

$$\theta \in CR^l \in \Theta \subseteq \Re^S, \tag{34.8}$$

where θ is treated as a vector of free variables and $\theta \in \mathrm{CR}^l$ indicates that θ is bounded in the regions given by CR^l, $N^{lk} = (n|y_n^{lk} = 1)$ and $P^{lk} = (n|y_n^{lk} = 0)$, and $|N^{lk}|$ is the cardinality of N^{lk} and K^l is the number of integer solutions that have already been analysed in CR^l. The formulation in (34) is a nonconvex problem which is solved to global optimality [4] by branching on x, y and θ and treating θ as a vector of free variables. The solution of (34) idenifies the next set of optimal integer variables by introducing the constraint, $f(x,y) \leqslant \hat{z}(\theta)^l$, to restrict the objective function to take values which are less than the current upper bound and introducing the integer cut, $y \neq \tilde{y}$, which is given by the constraint $\sum_{n \in N^{lk}} y_n^{lk} - \sum_{n \in P^{lk}} y_n^{lk} \leqslant |N^{lk}| - 1$, to eliminate the integer solutions that have already been analysed.

The integer vector obtained from the solution of (34) is then returned back to (33) to obtain another set of parametric profiles. Parametric solutions corresponding to two integer solutions are then compared and a lower envelope of the parametric solutions is retained by using the comparison procedure ([3], Appendix A) to update the current upper bound $z_{\tilde{y}}(\theta)$. The algorithm proceeds in this way until there is no feasible solution to (34) in each region in the space of θ. The final solution is given by the current upper bound $z_{\tilde{y}}(\theta)$.

4. Numerical Examples

In this section two examples are presented to illustrate the key steps of the algorithms presented earlier.

EXAMPLE 5. Consider Example 3. For illustration purposes, first few solution steps by using $\hat{z}_{O2}(\theta)$ and $\hat{z}_{O3}(\theta)$ are summarized in Table 2. For $\epsilon_1 = 0.01$ and $\epsilon_2 = 0$ and by using $\hat{z}_{O2}(\theta)$ the algorithm converges in 72 LPs (2.23 s), whereas 142 LPs (4.40 s) are solved when using $\hat{z}_{O3}(\theta)$, by using GAMS/CPLEX [12] on a Sun SPARC10-51 workstation. The final solution is given by:

$$z(\theta) = \begin{cases} 0.5\theta - 0.4922 \ \forall \theta \in [0, 0.5] \\ 0.1666\theta - 0.3255 \ \forall \theta \in [0.5, 1] \end{cases}$$

EXAMPLE 6. *Consider the following example which involves binary variables*:

$$z(\theta) = \min_{x,y} -x_1{}^2 - x_2{}^2 - y_1 - 2y_2 \tag{35.1}$$

$$s.t. \quad 4x_1{}^2 + x_1 + 3x_2{}^2 - y_1 + 10y_2 + 3\theta_1 - \theta_2 \leqslant 10 \tag{35.2}$$

$$2x_1{}^2 + 3x_2{}^2 + 2y_1 - y_2 - \theta_1 + 2\theta_2 \leqslant 16 \tag{35.3}$$

Table 2. Example 5: solution steps

Itn No.	x_1^R	x_2^R	θ_f	$\check{z}(\theta)$	$\hat{z}_{O2}(\theta)$	$\hat{z}_{O3}(\theta)$	Remarks
1	$[-1,1]$	$[-1,1]$	$[0,1]$	$0.5\theta-1$	0.5θ	1	(I) Branch on x_1^R. (II) Current upper bound: $\hat{z}_{O3}(\theta):1\forall\theta\in[0,1]$, $\hat{z}_{O2}(\theta):0.5\theta\forall\theta\in[0,1]$.
2(a)	$[-1,0]$	$[-1,1]$	$[0,1]$	$0.5\theta-0.5$	0.5θ	0	(I) Current upper bound: $\hat{z}_{O3}(\theta):0\forall\theta\in[0,1]$, $\hat{z}_{O2}(\theta):0.1\theta-0.1\forall\theta\in[0,1]$. (II) Branch on x_2^R.
2(b)	$[0,1]$	$[-1,1]$	$[0,1]$	$0.1\theta-0.6$	$0.1\theta-0.1$	$0.07143\theta+0.42857$	
3(a)	$[-1,0]$	$[-1,0]$	$[0]$	0	0.25	0	(I) Current upper bound: $\hat{z}_{O3}(\theta):0\forall\theta\in[0,1]$, $\hat{z}_{O2}(\theta)$: (i) $0.5\theta-0.5\forall\theta\in[0,0.5]$, (ii) $0.1666\theta-0.0833\forall\theta\in[0.5,1]$. (II) In (a) and (d) the underestimator crosses the current upper bound. (III) Fathom (a) and (d). Branch on x_1^R in (b) and (c).
3(b)	$[0,1]$	$[-1,0]$	$[0,1]$	$0.1666\theta-0.3333$	$0.1666\theta-0.0833$	0	
3(c)	$[-1,0]$	$[0,1]$	$[0,1]$	$0.5\theta-0.5$	$0.5\theta-0.25$	0	
3(d)	$[0,1]$	$[0,1]$	$[0,1]$	0	0.25	0.333θ	

x_1^R and x_2^R are the ranges of x_1 and x_2 respectively. θ_f is the feasible range of θ for the given x_1^R and x_2^R.

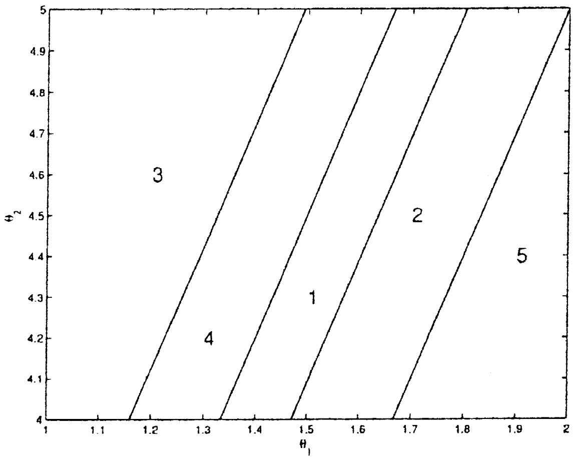

Figure 9. Critical Regions for Example 6.

Table 3. Parametric Solution of Example 6

S. No.	y	$z(\theta)$	Critical region
1	1,1	$0.3\theta_1 - 0.1\theta_2 - 3.125$	$-1.186\theta_1 + 0.395\theta_2 \geqslant -0.164$ $-1.2\theta_1 + 0.4\theta_2 \leqslant 0$
2	1,1	$1.486\theta_1 - 0.495\theta_2 - 3.289$	$-1.186\theta_1 + 0.395\theta_2 \leqslant -0.164$ $-3\theta_1 + \theta_2 \geqslant -1$
3	1,1	$0.773\theta_1 - 0.258\theta_2 - 3.25$	$-0.727\theta_1 + 0.242\theta_2 \geqslant 0.125$
4	1,1	$1.5\theta_1 - 0.5\theta_2 - 3.125$	$-0.727\theta_1 + 0.242\theta_2 \leqslant 0.125$ $-1.2\theta_1 + 0.4\theta_2 \geqslant 0$
5	1,0	-2.875	$-3\theta_1 + \theta_2 \leqslant -1$

$$0 \leqslant x_1 \leqslant 1 \tag{35.4}$$

$$0 \leqslant x_2 \leqslant 1 \tag{35.5}$$

$$1 \leqslant \theta_1 \leqslant 2 \tag{35.6}$$

$$4 \leqslant \theta_2 \leqslant 5. \tag{35.7}$$

The global solution of this problem by using the algorithms described in the previous section is given in Table 3 and the graphical interpretation of the critical regions is given in Figure 9. The algorithm requires a solution of 225 NLPs consuming 32.14 CPU seconds by using GAMS/CONOPT2 (for NLPs) [12] for $\epsilon_1 = \epsilon_2 = 0.25$ on a Sun SPARC10-51 workstation.

5. Concluding Remarks

In general, a local solution of a parametric nonconvex program does not provide a parametric overestimator (remarks 5–6). In this paper four different ways of obtaining a parametric overestimator were presented. The performance of the overestimators depends upon whether the problem is single or multiparametric (remarks 9–10) and also on whether the nonconvex terms are present in the objective function or the constraints (Lemmas 2, 3 and Remarks 11–13). The performance can be measured in terms of the effort required to obtain the overestimators, tightness of the overestimators and also the effort required to compare the overestimators to underestimators. This affects the overall performance of the algorithm as demonstrated with illustrations. A branch and bound algorithmic framework for the solution of multiparametric continuous and mixed-integer optimization problems has been presented and tested on examples.

Acknowledgements

Financial support from EPSRC (IRC Grant) and DETR/ETSU (Ref. no.: E/RD/00165/00/00/00/4473) is gratefully acknowledged. Thanks to Professor C. A. Floudas for his thoughtful suggestions from which the paper has benefited.

References

1. Acevedo, J. and Pistikopoulos, E. N. (1996), A parametric MINLP algorithm for process synthesis problems under uncertainty, *Industrial and Engineering Chemistry Research* 35, 147–158.
2. Acevedo, J. and Pistikopoulos, E. N. (1997a), A hybrid parametric/stochastic programming approach for mixed-integer linear problems under uncertainty, *Industrial and Engineering Chemistry Research* 36, 2262–2270.
3. Acevedo, J. and Pistikopoulos, E. N. (1997b), A multiparametric programming approach for linear process engineering problems under uncertainty, *Industrial and Engineering Chemistry Research* 36, 717–728.
4. Adjiman, C. S., Androulakis, I.P. and Floudas, C. A. (2000), Global optimization of mixed-integer nonlinear problems, *American Institute of Chemical Engineers Journal* 46, 1769–1797.
5. Adjiman, C. S., Dallwig, S., Floudas, C.A. and Neumaier, A. (1998), A global optimization method, αBB, for general twice-differentiable constrained NLPs – 1 Theoretical advances, *Computers & Chemical Engineering* 22, 1137–1158.
6. Androulakis, I. P., Maranas, C. D. and Floudas, C. A. (1995), α-BB: A global optimization method for general constrained nonconvex problems, *J. Global Optimization* 7, 337–363.
7. Bansal, V., Perkins, J. D. and Pistikopoulos, E. N. (2000a), Flexibility analysis and design of linear systems by parametric programming, *American Institute of Chemical Engineers Journal* 46, 335–354.
8. Bansal, V., Perkins, J. D. and Pistikopoulos, E. N. (2000b), Using mathematical programming to compute singular multivariate normal probabilities, *J. Stat. Comput. Simul.* 67, 219–253.
9. Bansal, V., Perkins, J. D. and Pistikopoulos, E. N. (2001), A unified framework for the flexibility analysis and design of non-linear systems via-parametric programming. In: Gani, R. and Jørgensen, S. B. (eds.), *European Symposium on Computer Aided Process Engineering-11*, pp. 961–966.

10. Bemporad, A., Morari, M., Dua, V. and Pistikopoulos, E. N. (2002), The explicit linear quadratic regulator for constrained systems, *Automatica* 38, 3–20.
11. Benson, H. P. (1982), Algorithms for parametric nonconvex programs, *J. of Optim. Theory Appl.* 38, 319–334.
12. Brooke, A., Kendrick, D. and Meeraus, A. (1998), *GAMS: A Users Guide*. California: Scientific Press.
13. Dua, V., Bozinis, N. A. and Pistikopoulos, E. N. (2002), A multiparametric programming approach for mixed-integer quadratic engineering problems, *Computers & Chemical Engineering* 26, 715–733.
14. Dua, V., Papalexandri, K. P. and Pistikopoulos, E. N. (1999), A parametric mixed-integer global optimization framework for the solution of process engineering problems under uncertainty, *Computers & Chemical Engineering* 23, S19–S22.
15. Dua, V. and Pistikopoulos, E. N. (1998), Optimization techniques for process synthesis and material design under uncertainty, *Transactions of IChemE* 76, 408–416.
16. Dua, V. and Pistikopoulos, E. N. (1999), Algorithms for the solution of multiparametric mixed-integer nonlinear optimization problems, *Industrial and Engineering Chemistry Research* 38, 3976–3987.
17. Dua, V. and Pistikopoulos, E. N. (2000), An algorithm for the solution of multiparametric mixed integer linear programming problems, *Annals of Operations Research* 99, 123–139.
18. Epperly, T. G. W. and Pistikopoulos, E. N. (1997), A reduced space branch and bound algorithm for global optimization, *J. Global Optimization* 11, 287–311.
19. Fiacco, A. V. (1983), *Introduction to Sensitivity and Stability Analysis in Nonlinear Programming.* New York: Academic Press.
20. Fiacco, A. V. (1990), Global multiparametric optimal value bounds and solution estimates for separable parametric programs, *Annals of Operations Research* 27, 381–396.
21. Floudas, C. A. (1999), *Deterministic Global Optimization: Theory, methods and applications*. Kluwer Academic Publishers, Dordrecht, The Netherlands.
22. Floudas, C. A., Pardalos, P. M., Adjiman, C. S., Esposito, W. R., Gümüs, Z. H., Harding, S. T., Klepeis, J. L., Meyer, C. A. and Schweiger, C. A. (1999), *Handbook of Test Problems in Local and Global Optimization*. Kluwer Academic Publishers, Dordrecht.
23. Floudas, C. A. and Visweswaran, V. (1990), A global optimization algorithm (GOP) for certain classes of nonconvex NLPs – I. Theory, *Computers & Chemical Engineering* 14(12), 1397–1417.
24. Gal, T. (1995), *Postoptimal Analyses, Parametric Programming, and Related Topics*. de Gruyter, New York.
25. Grossman, I. E. (1996), *Global Optimization in Engineering Design.* Kluwer Academic Publishers, Dordrecht, The Netherlands.
26. Hené, T. S. , Dua, V. and Pistikopoulos, E. N. (2002), A hybrid parametric/stochastic programming approach for mixed-integer nonliner problems under uncertainty, *Industrial and Engineering Chemistry Research* 41, 67–77.
27. Horst, R. and Tuy, H. (1996), *Global Optimization: Deterministic approaches*. Kluwer Academic Publishers, Dordrecht.
28. Kakalis, N. M. P. (2001), Robust model predictive control via parametric programming, Master's thesis, Imperial College, London, U.K.
29. Kakalis, N. P., Dua, V., Sakizlis, V., Perkins, J. D. and Pistikopoulos, E. N. (2002), A parametric optimisation approach for robust MPC. presented at the 15th IFAC World Congress on Automatic Control, Barcelona, 2002.
30. Konno, H. and Yajima, Y. (1991), Parametric simplex algorithms for solving a special class of nonconvex minimization problems, *J. Global Optimization* 1(1), 65–81.
31. Kosmidis, V. S. (1999), Multiparametric analysis of mixed integer linear programming problems. Master's thesis, Imperial College, London, U.K.

32. McCormick, G. P. (1976), Computability of global solutions to factorable nonconvex programs: Part I – Convex underestimating problems, *Math. Progr.* 10, 147–175.
33. Papalexandri, K. and T. Dimkou (1998), A parametric mixed integer optimization algorithm for multi-objective engineering problems involving discrete decisions, *Industrial and Engineering Chemistry Research* 37(5), 1866–1882.
34. Pertsinidis, A. (1992), On the parametric optimization of mathematical programs with binary variables and its application in the chemical engineering process synthesis. Ph.D. thesis, Carnegie Mellon University, Pittsburgh, PA, USA.
35. Pertsinidis, A., Grossmann, I. E. and McRae, G. J. (1998) Parametric optimization of MILP programs and a framework for the parametric optimization of MINLPs, *Computers and Chemical Engineering* 22, S205.
36. Pistikopoulos, E. N. (1997), Parametric and stochastic programming algorithms for process synthesis, design and optimization under uncertainty. Presented at Aspen World, Boston, Massachusetts.
37. Pistikopoulos, E. N., Bozinis, N. A. and Dua, V. (1999), POP: A MATLAB (© The Math Works, Inc.) implementation of multi-parametric quadratic programming algorithm. Centre for Process Systems Engineering, Imperial College.
38. Pistikopoulos, E. N., Bozinis, N. A. and Dua, V. (2000a), A MATLAB (© The Math Works, Inc.) implementation of multi-parametric mixed-integer linear programming algorithm. Centre for Process Systems Engineering, Imperial College.
39. Pistikopoulos, E. N. and Dua, V. (1998), Planning under uncertainty: a parametric optimization approach. In: J. F. Pekny and G. E. Blau (eds) *Proc. Third International Conference on Foundations of Computer-Aided Process Operations*, pp. 164–169.
40. Pistikopoulos, E. N., Dua, V., Bozinis, N. A., Bemporad, A. and Morari, M. (2000), On-line optimization via off-line parametric optimization tools, *Computers & Chemical Engineering* 24, 183–188.
41. Pistikopoulos, E. N., Dua, V., Bozinis, A., Bemporad, A. and Morari, M. (2002), On-line optimization via off-line parametric optimization tools, *Computers & Chemical Engineering* 26, 175–185.
42. Pistikopoulos, E. N. and Grossmann, I. E. (1988), Optimal retrofit design for improving process flexibility in linear systems, *Computers & Chemical Engineering* 12(7), 719–731.
43. Quesada, I. and Grossmann, I. E. (1995), A global optimization algorithm for linear fractional and bilinear programs, *J. Global Optimization* 6, 39–76.
44. Ryu, J. and E. N. Pistikopoulos: (2001), Solving scheduling problems under uncertainty using parametric programming. In: Stephanopoulos, G., Lee, J. H. and Yoon, E. S. (eds), *Proc. 6th IFAC Symposium on Dynamics and Control of Process Systems*. pp. 225–230.
45. Sakizlis, V., Dua, V., Kakalis, N., Perkins, J. D. and Pistikopoulos, E. N. (2001a), The explicit control law for hybrid systems via parametric programming. In: Kovács, G. L. (ed.), *IFAC Workshop on Manufacturing, Modelling, Management and Control* pp. 128–133.
46. Sakizlis, V., Dua, V., Kakalis, N., Perkins, J. D. and Pistikopoulos, E. N. (2002a), Robust model-based controllers via parametric programming. In: J. Grievink and J. van schijndel (eds.), *Proceedings of the 12th European Symposium on Computer-Aided Process En gineering.* pp. 541–546.
47. Sakizlis, V., Dua, V., Perkins, J. D. and Pistikopoulos, E. N. (2001b), Algorithms for the solution of multiparametric dynamic and mixed integer programs, presented at Annual AIChE meeting, Reno.
48. Sakizlis, V., Dua, V., Perkins, J. D. and Pistikopoulos, E. N. (2001c), The explicit model based control law for process systems via parametric programming. In: C. E. D'Attellis, Kluev, V. V. and Mastorakis, N. E. (eds.) *Mathematics and Simulation with Biological , Economical and Musicoacoustical Applications,* ISBN 960-8052-46-7. pp. 253–259.

49. Sakizlis, V., Dua, V., Perkins, J. D. and Pistikopoulos, E. N. (2001d), An explicit model based control law for hybrid dynamic systems via multiparametric mixed integer programming, presented at Annual AIChE meeting, Reno.
50. Sakizlis, V., Dua, V., Perkins, J. D. and Pistikopoulos, E. N. (2001e), The explicit MPC-based feedback control law via parametric programming. presented at Annual AIChE meeting, Reno.
51. Sakizlis, V., Dua, V., Perkins, J. D. and Pistikopoulos, E. N. (2002b), The explicit control law for hybrid systems via parametric programming. Proceedings of the 2002 American Control Conference, Anchorage, pp. 674–679.
52. Sakizlis, V., Dua, V., Perkins, J. D. and Pistikopoulos, E. N. (2002c), The explicit model-based control law for continuous time systems via parametric programming. Proceedings of the 2002 American Control Conference, Anchorage, pp. 4501–4506.
53. Sakizlis, V., Perkins, J. D. and Pistikopoulos, E. N. (2001f), An algorithm for multiparametric dynamic optimization. submitted to ICOTA'01, Hong Kong.
54. Sakizlis, V., Perkins, J. D. and Pistikopoulos, E. N. (2001g), Multiparametric dynamic optimization of linear quadratic optimal control problems: theory and applications. In: Luus, R. (ed.), *Recent Developments in Optimization and Optimal Control in Chemical Engineering,* accepted. Research Signpost.

Appendix

A. COMPARISON OF PARAMETRIC SOLUTIONS

[3] proposed an approach for comparing two parametric solutions, $z(\theta)^1$ and $z(\theta)^2$, which are valid in the critical regions CR^1 and CR^2 respectively. Their approach, which consists of two steps, is briefly described here. The first step is to define a region, $\mathrm{CR}^{\mathrm{int}} = \mathrm{CR}^1 \cap \mathrm{CR}^2$, where both the parametric solutions are valid. $\mathrm{CR}^{\mathrm{int}}$ can be defined by removing all the redundant constraints from the set of inequalities which define CR^1 and CR^2 – for a procedure to identify redundant constraints, see [24]. In the second step, check: if $\mathrm{CR}^{\mathrm{int}} = \emptyset$, then $z(\theta)^1$ and $z(\theta)^2$ are the solutions in CR^1 and CR^2, respectively, otherwise a new constraint, $z(\theta)^1 \leqslant z(\theta)^2$, is formulated and a constraint redundancy check is made for the new constraint in $\mathrm{CR}^{\mathrm{int}}$. This constraint redundancy test results in three cases which are analyzed as follows:

Case 1: If the new constraint is redundant, then $z(\theta)^1 \leqslant z(\theta)^2$, $\forall \theta \in \mathrm{CR}^{\mathrm{int}}$.
Case 2: If the new constraint is infeasible, then $z(\theta)^1 \geqslant z(\theta)^2$, $\forall \theta \in \mathrm{CR}^{\mathrm{int}}$.
Case 3: If the new constraint is non-redundant, then:

- $z(\theta)^1 \leqslant z(\theta)^2, \forall \theta \in \Delta\{\vec{\mathrm{CR}}^{\mathrm{int}}, z(\theta)^1 - z(\theta)^2 \leqslant 0\}$, AND
- $z(\theta)^1 \geqslant z(\theta)^2, \forall \theta \in \Delta\{\vec{\mathrm{CR}}^{\mathrm{int}}, z(\theta)^1 - z(\theta)^2 \geqslant 0\}$

where Δ is an operator which removes redundant constraints and $\vec{\mathrm{CR}}^{\mathrm{int}}$ represents the set of constraints which define $\mathrm{CR}^{\mathrm{int}}$. To identify the regions $\mathrm{CR}^1 - \mathrm{CR}^{\mathrm{int}}$ and $\mathrm{CR}^2 - \mathrm{CR}^{\mathrm{int}}$ use the procedure described in Appendix B [17].

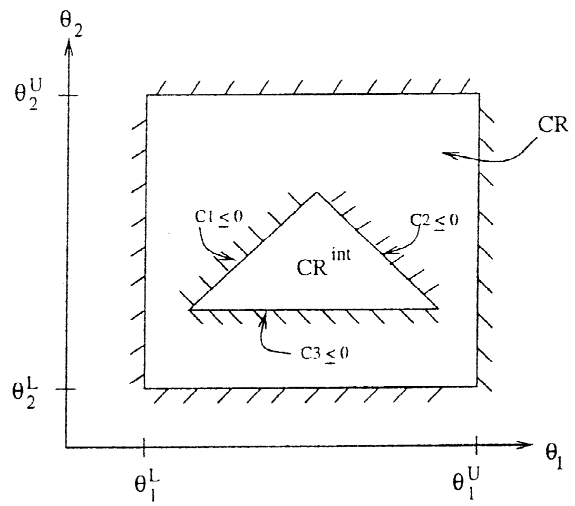

Figure 10. Critical regions, CR and CR^{int}.

Table 4. Definition of rest of the regions

Region	Inequalities
CR_1^{rest}	$C1 \geqslant 0, \theta_1^L \leqslant \theta_1, \theta_2 \leqslant \theta_2^U$
CR_2^{rest}	$C1 \leqslant 0, C2 \geqslant 0, \theta_1 \leqslant \theta_1^U, \theta_2 \leqslant \theta_2^U$
CR_3^{rest}	$C1 \leqslant 0, C2 \leqslant 0, C3 \geqslant 0, \theta_1^L \leqslant \theta_1 \leqslant \theta_1^U, \theta_2^L \leqslant \theta_2$

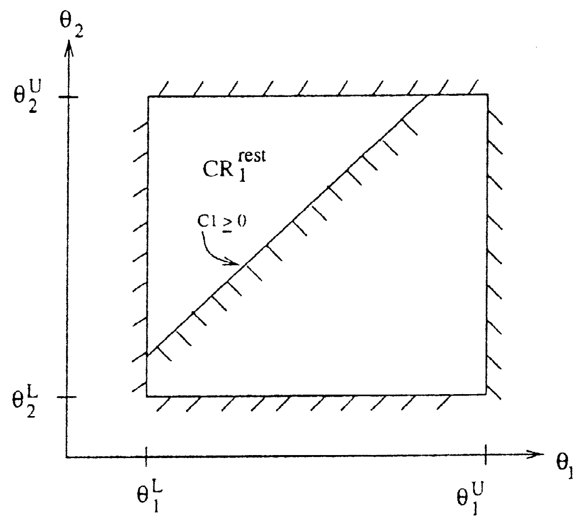

Figure 11. Division of critical regions – Step 1.

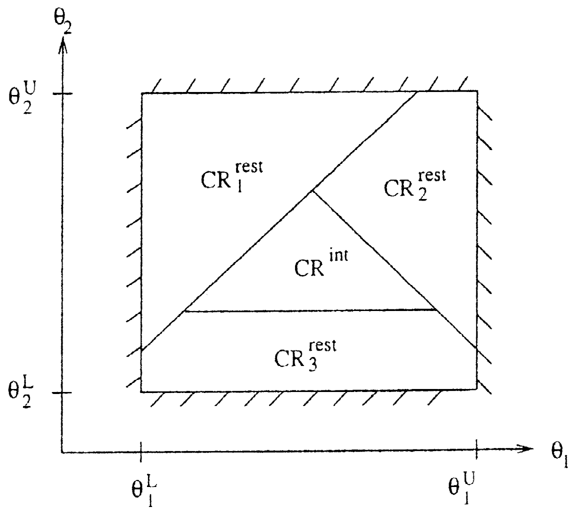

Figure 12. Division of critical regions – rest of the regions.

B. DEFINITION OF REST OF THE REGION

Given an initial region, CR and a feasible region, $\mathrm{CR}^{\mathrm{int}}$ such that $\mathrm{CR}^{\mathrm{int}} \subseteq \mathrm{CR}$, a procedure is described in this section to define the rest of the region, $\mathrm{CR}^{\mathrm{rest}} = \mathrm{CR} - \mathrm{CR}^{\mathrm{int}}$. For the sake of simplifying the explanation of the procedure, consider the case when only two parameters, θ_1 and θ_2, are present (see Figure 10), where CR is defined by the inequalities: $\{\theta_1^L \leqslant \theta_1 \leqslant \theta_1^U, \theta_2^L \leqslant \theta_2 \leqslant \theta_2^U\}$ and $\mathrm{CR}^{\mathrm{int}}$ is defined by the inequalities: $\{C1 \leqslant 0, C2 \leqslant 0, C3 \leqslant 0\}$ where $C1$, $C2$ and $C3$ are linear in θ. The procedure consists of considering one by one the inequalities which define $\mathrm{CR}^{\mathrm{int}}$. Considering, for example, the inequality $C1 \leqslant 0$, the rest of the region is given by, $\mathrm{CR}_1^{\mathrm{rest}}: \{C1 \geqslant 0, \theta_1^L \leqslant \theta_1,\ \theta_2 \leqslant \theta_2^U\}$, which is obtained by reversing the sign of inequality $C1 \leqslant 0$ and removing redundant constraints in CR (see Figure 11). Thus, by considering the rest of the inequalities, the complete rest of the region is given by: $\mathrm{CR}^{\mathrm{rest}} = \{\mathrm{CR}_1^{\mathrm{rest}} \cup \mathrm{CR}_2^{\mathrm{rest}} \cup \mathrm{CR}_3^{\mathrm{rest}}\}$, where $\mathrm{CR}_1^{\mathrm{rest}}$, $\mathrm{CR}_2^{\mathrm{rest}}$ and $\mathrm{CR}_3^{\mathrm{rest}}$ are given in Table 4 and are graphically depicted in Figure 12.