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Abstract

Mathematical programming methods have been applied to study equilibrium refueling of nuclear reactors. In particular fuel management problems are solved by successive linearization. The domain of validity of these approximations is specified by a quadratic spherical constraint. The approach proposed in this paper involves the reformulation of each problem and the use of parametric linear complementarity theory to solve it. Numerical results are included to demonstrate the efficiency of the approach and compare it with the augmented Lagrangian method.

1. Introduction

Mathematical programming methods have been used to study the equilibrium refueling of nuclear reactors. The problem is to minimize the total reactor feed rate under equilibrium refueling by adjusting the exit irradiation of the fuel in specified burnup zones under some constraints on excess reactivity and on the power shape in the reactor. This problem is solved using successive linearizations of the objective and constraint functions (see [3,9]). The method of approximate programming (MAP) proposed by Griffiths et al. [4] (also analyzed in [8]) requires a linear programming problem to be solved at each iteration, but upper and lower bounds are added on variables to limit their variation inside a domain of validity of the approximation:

$$\begin{aligned} \text{Min} \quad & c^T x \\ \text{Subject to} \quad & Ax \le b \\ & \ell \le x \le u \end{aligned} \tag{1.1}$$

where $c, \ell, u, x \in E^n$, $b \in E^m$ and A is an mxn matrix.

To reduce the number of linearizations required to solve the problem, it was proposed in [3] to use a quadratic constraint of the form $\frac{1}{2}x^T Px \le d$ rather than upper and lower bounds on individual variables. This, in fact, reduces the "extremality" effect of linear programming by smoothing a rectangular constraint in (MAP) by a ~~special~~ spherical constraint. The linearizations take the form:

$$\begin{aligned} \text{Min} \quad & c^T x \\ \text{Subject to} \quad & Ax \le b \\ & \tfrac{1}{2}x^T Px \le d \end{aligned} \tag{1.2}$$

where P is a positive definite matrix of order n.

Several techniques are available to solve such a problem (in particular the augmented Lagrangian approach as implemented in MINOS [6]), but we rather propose to reformulate the problem and to use parametric linear complementarity theory to solve it. This approach is presented in Section 2. In Section 3 the algorithm is presented and in Section 4 the problem with non negative constraints on the variables is analyzed. Finally, Section 5 includes numerical results.

2. Parametric linear complementarity approach

In the first step of the procedure, the relaxed problem:

$$\begin{aligned} \text{Min} \quad & c^T x \\ \text{Subject to} \quad & Ax \le b \end{aligned} \tag{2.1}$$

is solved. Assume that $z^* > (-\infty)$ is the optimal value and that x^* is an optimal solution of (2.1). It is well known that if x^* satisfies the constraint $\frac{1}{2} x^{*T} P x^* \le d$, then x^* is an optimal solution of (1.2), and the procedure stops. Otherwise, there exists an optimal solution of (1.2) for which the additional constraint holds with equality. Hence, rather than solving (1.2), consider the following problem

$$\begin{aligned} \text{Min} \quad & \tfrac{1}{2} x^T P x \\ \text{Subject to} \quad & Ax \le b \\ & c^T x \le z^* + \tau . \end{aligned} \tag{2.2}$$

It is easy to verify that (1.2) is equivalent to determining the smallest value $\tau^* \ge 0$ such that an optimal solution $\bar{x}$ of (2.2) with $\tau = \tau^*$ satisfies $\frac{1}{2} \bar{x}^T P \bar{x} = d$ and $c^T \bar{x} = z^* + \tau^*$. Indeed, for $\tau = 0$, x^* is a feasible solution of (2.2) where $\frac{1}{2} x^* P x^* > d$, and the optimal value of (2.2) is a non-increasing function of τ because the feasible domain can only get larger as τ increases.

The Kuhn-Tucker first order optimality conditions for (2.2) are given as follows:

$$Px + A^T\nu + \pi c = 0 \tag{2.3}$$

$$\nu^T(b-Ax) = 0$$

$$\pi(z^* + \tau - c^T x) = 0$$

$$Ax \le b \tag{2.4}$$

$$c^T x \le z^* + \tau \tag{2.5}$$

$$\nu \ge 0,\ \pi \ge 0.$$

Since P is a positive definite matrix, from (2.3) it follows that

$$x = -P^{-1}A^T\nu - \pi P^{-1}c. \tag{2.6}$$

Substituting this value of x in (2.4) and (2.5),

$$0 \le b - Ax = b + AP^{-1}A^T\nu + \pi AP^{-1}c \qquad = w \tag{2.7}$$

$$0 \le z^* + \tau - c^T x = z^* + \tau + c^T P^{-1}A^T\nu + c^T P^{-1}c = \alpha. \tag{2.8}$$

This system can be written in matrix form as

$$\begin{bmatrix} w \\ \\ \alpha \end{bmatrix} = \begin{bmatrix} b \\ \\ z^* \end{bmatrix} + \tau \begin{bmatrix} 0 \\ \\ 1 \end{bmatrix} + \begin{bmatrix} AP^{-1}A^T & AP^{-1}c \\ \\ c^T P^{-1}A^T & c^T P^{-1}c \end{bmatrix} \begin{bmatrix} \nu \\ \\ \pi \end{bmatrix} \tag{2.9}$$

$$w \ge 0,\ \alpha \ge 0. \tag{2.10}$$

Including the non-negativity conditions

$$\nu \ge 0,\ \pi \ge 0 \tag{2.11}$$

and the complementarity condition

$$w^T\nu + \alpha\pi = 0, \tag{2.12}$$

we obtain an equivalent system to the Kuhn-Tucker conditions for problem (2.2).

The approach involves solving the parametric (in τ) linear complementarity problem (2.9) - (2.12) until we identify the smallest value of the parameter $\tau^* > 0$ such that the corresponding value $\bar{x}$ satisfies $\frac{1}{2}\bar{x}^T P\bar{x} = d$ and $c^T\bar{x} = z^* + \tau^*$.

Now, suppose that problem (2.1) is unbounded below. To handle this case as before, we have to select a point x^* on the extreme ray identified at the last iteration of the simplex with a value $z^* = c^T x^*$ small enough to ensure that the optimal value of (2.2) where $\tau = 0$ is larger than or equal to d. Indeed, otherwise the optimal value of (1.2) might be smaller than z^* and the procedure could not identify it.

3. Algorithm

To simplify the statement of the algorithm, denote

$$M = \begin{bmatrix} AP^{-1}A^T & AP^{-1}c \\ c^TP^{-1}A^T & c^TP^{-1}c \end{bmatrix}, \quad q = \begin{bmatrix} b \\ z^* \end{bmatrix}, \quad p = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad y = \begin{bmatrix} w \\ \alpha \end{bmatrix}, \quad t = \begin{bmatrix} \nu \\ \pi \end{bmatrix} .$$

Then the parametric linear system (2.9) can be written

$$y = q + \tau p + Mt \quad . \tag{3.1}$$

The algorithm is summarized as follows:

Step 1. Solve the relaxed problem (2.1). If $z^* < -\infty$, let x^* be an optimal solution. If $\frac{1}{2}x^{*T}Px^* \le d$, then x^* is an optimal solution of (1.1) and the procedure terminates. Otherwise, let FL=0 and move to Step 2.

If (2.1) is unbounded below, select x^* on the extreme ray identified at the last iteration of the simplex procedure such that $x^{*T}Px^* > d$. Let FL=1 and $z^* = c^Tx^*$.

Step 2. Specify the system (3.1) using z^*. Determine a complementary solution of (3.1) with $\tau = 0$ using a complementary pivot algorithm and performing the pivots on column p also. The transformed system is denoted

$$g = \bar{q} + \tau\bar{p} + \bar{M}h. \tag{3.2}$$

Denote by x(0) the corresponding value of x.

If $\frac{1}{2}x(0)^T Px(0) > d$, let $\tau\ell = 0$, val = $\frac{1}{2}x(0)^T Px(0)$, and move to Step 3. Otherwise, if FL = 0 , then $\frac{1}{2}x(0)^T Px(0) = d$, and x(0) is an optimal solution of (1.1) and the procedure terminates. If FL=1, select a new point x* on the extreme ray identified at the last iteration of the procedure such that its value z* is twice as small as before. Repeat Step 2.

<u>Step 3</u>. If $\bar{p} \geq 0$, then move to Step 6.

<u>Step 4</u>. Let

$$\tau\ell = -\frac{\bar{q}_r}{\bar{p}_r} = \text{Min}\left\{-\frac{\bar{q}_i}{\bar{p}_i} : \bar{p}_i < 0\right\}.$$

Evaluate val = $\frac{1}{2}x(\tau\ell)^T Px(\tau\ell)$.

<u>Step 5</u>. If val $\leq$ d, move to Step 6.

If $\bar{m}_{rr} > 0$, pivot on $\bar{m}_{rr}$ to obtain a new system of the form (3.2). Repeat Step 3.

If $\bar{m}_{rr} = 0$, determine the index s such that

$$-\frac{1}{m_{sr}}\left[\bar{q}_s - \frac{\bar{p}_s}{\bar{p}_r}\bar{q}_r\right] = \text{Min}\left\{-\frac{1}{m_{ir}}\left[\bar{q}_i - \frac{\bar{p}_i}{\bar{p}_r}\bar{q}_r\right] : m_{ir} < 0\right\}.$$

Execute a 2x2 block pivot on m_{rs} and m_{sr} to obtain a new system of the form (3.2). Repeat Step 3.

<u>Step 6</u>. Determine τ^* such that $\frac{1}{2}x(\tau^*)^T P\, x(\tau^*) = d$ using the variable x as a function of τ specified at $\tau\ell$. Then $x(\tau^*)$ is an optimal solution of (1.1), and the procedure terminates. □

Step 4 and 5 are the general steps of a parametric linear complementarity algorithm described by Cottle in [1]. This algorithm can be used because the matrix $\bar{M}$ is positive semi-definite.

Theorem 3.1 The matrix $\bar{M}$ defined in the algorithm is positive semi-definite.

Proof. First, it is easy to verify that the matrix M is positive semi-definite. Indeed the quadratic form

$$\mu^T M \mu = \begin{bmatrix}\rho^T, \gamma\end{bmatrix} \begin{bmatrix} AP^{-1}A^T & AP^{-1}c \\ c^T P^{-1} A^T & c^T P^{-1} c \end{bmatrix} \begin{bmatrix}\rho \\ \gamma\end{bmatrix} = \begin{bmatrix}\rho^T A + \gamma c^T\end{bmatrix} P^{-1} \begin{bmatrix}A^T \rho + \gamma c\end{bmatrix} \geq 0$$

since P is positive definite.

The result follows from [2,Theorem 2] since $\bar{M}$ is a principal transform of M (i.e. $\bar{M}$ is obtained from M via a block pivot on a principal submatrix of M). □

Furthermore, in Step 5, for the case were $\bar{m}_{rs} = 0$ there exists at least one index i such that $\bar{m}_{ir} < 0$. Indeed, if $m_{ir} \geq 0$ for all i, then $m_{ri} \leq 0$ for all i (see [2,Theorem 3]). Hence the parametric linear complementary system (3.1) would not have any solution for $\tau > \tau \ell$. This is a contradiction since (2.9) - (2.12) is equivalent to the Kuhn-Tucker conditions of problem (2.2) which has an optimal solution for all $\tau \geq 0$.

It is worth noticing that the quadratic form $x^T P x$ can be evaluated in terms of the variables ν, π and τ. Indeed, using (2.3),

$$\begin{aligned} x^T P x &= [\nu^T A P^{-1} + \pi c^T P^{-1}] \; P \; [P^{-1} A^T \nu + \pi P^{-1} c] \\ &= [\nu^T, \pi] \begin{bmatrix} AP^{-1}A^T & AP^{-1}c \\ c^T P^{-1} A^T & c^T P^{-1} c \end{bmatrix} \begin{bmatrix}\nu \\ \pi\end{bmatrix} \\ &= [\nu^T, \pi] \left\{ \begin{bmatrix} w \\ \alpha \end{bmatrix} - \begin{bmatrix} b \\ z^* \end{bmatrix} - \tau \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\} \qquad \text{(by (3.1))} \end{aligned}$$

$$= - [\ \nu^T, \pi\ ] \begin{bmatrix} b \\ z* + \tau \end{bmatrix} \qquad \text{(by (2.10))}$$

As a consequence,

$$\tfrac{1}{2}\ x(\tau)^T\ Px(\tau) = - \tfrac{1}{2}\{\nu(\tau)^T\ b + \pi(\tau)\ (z* + \tau)\}.$$

Furthermore, $\tau*$ is a solution of the equation

$$- \tfrac{1}{2}\{\nu(\tau)^T\ b + \pi(\tau)\ (z* + \tau)\} - d = 0$$

where the expression $\gamma(\tau)$ and $\pi(\tau)$ are those specified for $\tau = \tau\ell$.

4. Problem with non-negative variables

If problem (1.2) includes non-negative variables, then it can be formulated as

$$\begin{aligned} &\text{Min} \quad c^T x \\ &\text{Subject to} \quad Bx \le f \\ &\qquad -Ix \le 0 \\ &\qquad \tfrac{1}{2}x^T Px \le d \end{aligned} \qquad (4.1)$$

Hence using the notation of problem (1.2), it follows that

$$A = \begin{bmatrix} B \\ -I \end{bmatrix} \quad \text{and} \quad b = \begin{bmatrix} f \\ 0 \end{bmatrix} .$$

One way of solving problem (4.1) is to use the algorithm given in Section 3. But, referring to the Kuhn-Tucker conditions of (4.1), it can also be solved using the algorithm of Section 3 where

$$M = \begin{bmatrix} P & B^T & c \\ -B & 0 & 0 \\ -c^T & 0 & 0 \end{bmatrix}, \ q = \begin{bmatrix} 0 \\ f \\ z* \end{bmatrix}, \ p = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \ y = \begin{bmatrix} w_1 \\ w_2 \\ \beta \end{bmatrix}, \ t = \begin{bmatrix} x \\ \nu_2 \\ \pi \end{bmatrix} .$$

The same analysis as in Section 3 follows, except for the evaluation of $x^T Px$. It follows directly from the Kuhn-Tucker conditions that

$$\tfrac{1}{2}x^T Px = \tfrac{1}{2}[\nu_2^T f + \pi(z^* + \tau)] \ .$$

Consequently, τ^* in Step 6 is a solution of the equation

$$-\tfrac{1}{2}[\nu_2(\tau)^T f + \pi(\tau)\ (z^* + \tau)] - d = 0$$

where the expressions $\nu_2(t)$ and $\pi(\tau)$ are those specified for $\tau = \tau\ell$.

5. Numerical results

The purpose of the following tests is to verify the numerical potential of the approach. We did not make any specific effort to generate the most efficient computer code to implement the approach, but we rather used experimental computer codes available for Lemke's algorithm [7] and for linear programming [5]. These tests have been obtained with a CYBER 173 at the University of Montreal.

Five different problems were generated with a 10x30 constraint matrix A and three with a 15x50 constraint matrix A. The parameters were generated randomly as follows: $0 \le a_{ij} \le 10$, $-25 \le c_j \le 0$, $0 \le p_{ii} \le 10$. Furthermore, the density of A (i.e. the percentage of non-zero elements) was taken equal to 40%. For each of these problems three different values of d were tested. The results are summarized in TABLE 5.1 where the average CPU times for each variant are given. (Variant 1 is presented in Section 3 and variant 2 in Section 4). Note that the linear programming algorithm in [5] was used to solve problem (2.1) in both variants.

Problem size	Values of d	Variant 1	Variant 2	MINOS
10x30	5000	4.193	4.119	5.290
	3000	4.355	4.270	6.036
	1000	4.948	4.541	8.194
15x50	5000	12.232	12.897	10.461
	3000	13.079	13.663	11.820
	1000	14.167	14.909	18.037

TABLE 5.1

The tests indicate that the approach is competitive with MINOS. Furthermore, both variants are less sensitive to smaller values of d (thighter problems) than MINOS. Hence they become more efficient in these cases. Both variants seem equally efficient on the problems tested. In conclusion, these preliminary results show the adequacy of the approach for this problem.

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