A Penalty Function Approach for Solving Bi-Level Linear Programs

D. J. WHITE

Department of Decision Theory, University of Manchester, U.K.

and

G. ANANDALINGAM Department of Systems, University of Pennsylvania, U.S.A.

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Abstract. The paper presents an approach to bi-level programming using a duality gap-penalty function format. A new exact penalty function exists for obtaining a global optimal solution for the linear case, and an algorithm is given for doing this, making use of some new theoretical properties. For each penalty parameter value, the central optimisation problem is one of maximising a convex function over a polytope, for which a modification of an algorithm of Tuy (1964) is used. Some numerical results are given. The approach has other features which assist the actual decisionmaking process, which make use of the natural roles of duality gaps and penalty parameters. The approach also allows a natural generalization to nonlinear problems.

Key words. Bi-level programming, penalty function, non-convex optimisation.

1. Introduction

There has been much activity since the early 1980s in bi-level programming (BLP) which may be thought of as a static version of Stackelberg leader-follower games [22]. In several fields ranging from economics to transportation engineering, researchers used BLPs to model problems involving multiple decision makers, These problems include organizational design [2], spatial competition [16], facility location [23], signal optimization [19], and traffic assignment [9].

In BLP, the higher level decision maker (the leader) controls decision vector $x \in X \subseteq R^{n1}$ in order to solve an outer problem consisting of maximizing his objective F(x, y), where $y \in Y \subseteq R^{n2}$ is the lower level (follower's) decision vector. For r followers, $y = (y_1, \ldots, y_r)$ and $n2 = \sum n_i$ where n_i is the dimension of the *i*-th follower's decision variable. For a given x = x', the inner problem consists of the follower maximizing his objective function f(x', y) to obtain $y' \in RR(x')$ where $RR(\cdot)$ is the rational reaction function of the follower.

A problem with bi-level mathematical programs is that they are non-convex. There are two main approaches to solve bi-level linear programming problems: enumeration techniques including implicit enumeration [11], and the "k-th best" algorithm [10], and the Kuhn-Tucker approach which is solved by mixed integer programming [13], grid search [5], and parametric complementary pivoting [10, 18]. While these approaches try to handle the nonconvexity, it is well known

that the popular Bard's grid search and Bialas and Karwan's parametric complementary pivoting methods only find local minima. In a recent paper, Anandalingam *et al.* [3] use simulated annealing and genetic algorithm based approaches to obtain global solutions to the bi-level linear program.

In this paper, we provide an algorithm, based on a penalty function approach, for solving bi-level linear programming problems. This work uses an alternative format to that of Bard [6], and is based on the work of Anandalingam and White [4]. For a given x, the leader's decision vector, the follower is at his rational reaction set when the duality gap of the second level problem becomes a zero. The outer problem is solved by appending to the leader's objective function, a function that minimizes the duality gap of the follower's problem. Although the hybrid objective function is nonlinear, it can be decomposed to provide a set of linear programs conditioned on either the decision vectors (x, y), or the dual vectors w of the follower's problem. There is an exact penalty function that yields the global optimal solution, which provides a finite algorithm for extracting it by solving a series of linear programs. The paper of Bard [6] also uses a penalty function approach. Although there is some common ground with the current paper, the content and objective of Bard's paper are somewhat distinct from those of the current paper. The penalty part of Bard's paper does offer an alternative penalty formulation and the paper is of sufficient significance to be addressed as a special issue. This is done in Section 6 in our paper.

There are related papers by Shimizu and Aiyoshi [21] and Aiyoshi and Shimizu [1] that use a penalty function approach for solving nonlinear bi-level programming problems. These papers are significantly different from ours. In their paper, the objective functions of the leader and follower are nonlinear and the penalty function is convex, facilitating the use of the conjugate gradient method. In addition, they solve for local, rather than global, optima. Also, the proposed method solves a sequence of linear programs which is easier to use than the methods proposed by Shimizu and Aiyoshi [21].

The contributions of the paper are as follows

- (i) A new global optimization penalty function method is presented for the linear bi-level programming problem. This is done in Section 3.
- (ii) A comparison is made with the penalty function method of Bard [6], and it is demonstrated that the proposed penalty formulation has some qualitative advantages over that of Bard [6]. This is done in Section 6.
- (iii) The penalty function-duality gap approach gives a natural way of capturing the optimality conditions of the follower in a manner which allows mathematical characteristics to be used, and the impact of deviations from optimality to be evaluated. This is explored in Section 5, where the significance of solving the penalty scalar optimization problem for any given value of the penalty parameter K is explored in the context of the decisionmaking process involved.

- (iv) Although expressions for values of K large enough to lead to actual optima are given in Section 6, it remains an open question as to how such K may be computed. Thus, at this stage of the work, we can only select some K to begin with and to increase K until we achieve an optimal solution, or a satisfactory solution, using the results of Section 5 if desired. It is of some computational advantage not to insist on K being too large because of possible computational instabilities.
- (v) Another advantage of the penalty function-duality gap approach is that the multi-decisionmaker, multi-level, problem is also reducible to a single penalty factor scalar optimization problem. Although we have not done this, it does offer an approach to even more complex problems, without adding more complexity to the approach than that arising from the number of variables involved.
- (vi) It is possible to extend the penalty function-duality gap approach to some non-linear bi-level problems, and this is done in Section 6. It is not possible to extend the approach of Bard [6] in the same way. Some of the results at the linear case will still hold. This is done in Section 6.
- (vii) Some algorithmic and computational results are given in Sections 3 and 4 for the linear case. The algorithm used is essentially that of Tuy [24] modified to cope with degeneracy (an unlikely event), and with cycling, and supplemented with some theoretical devices via Theorems 5-8. Theorems 6-7 are new and give useful results in cases when positive or negative correlation between the objective functions of the decisionmakers arises. It is established that the computational results using the modified method of Tuy are not as good as these of Bard [6]. The problem of maximizing a convex function over a polytope is a hard one, whichever method is used. There are other methods which we have not explored. The theoretical appeal of the penalty function-duality gap approach as outlined in the earlier paragraphs seems, at this stage, to explore other methods, which may be able to exploit the particular structure of the problem. The function $\hat{F}(\cdot, \cdot, \cdot, K)$, is a bi-linear function for which methods exist. Indeed, the proposed method is a method for solving any bi-linear problem. Other methods may be found, for example, in Horst and Tuy [17].
- (viii) Theorems 6–8 of Section 3.3 are geared to finding starting solutions for the algorithm, whose goodness will depend upon the degree of correlation between the objectives. However, the bounds given are usable in a branch and bound mode. The same applies to the loss of optimality bounds developed in Section 5 for other purposes.
- (ix) Finally we note that the singleton requirement A1 is weaker than the usual requirement made in other algorithms, in that it is required to apply only for optimal solutions. This is somewhat more reasonable to accept in practice. It is only required to get the exact penalty result.

2. The Bi-Level Programming Problem

Let us consider a two-level hierarchical system where the higher level decision maker, the leader, controls decision vector $x \in X$, and the lower level decision maker, the follower, controls decision vector $y \in Y$. The leader is assumed to select a decision vector first, and the follower to select a decision vector after that. In order to formulate the problem, let us define the following:

$$X = \text{a closed convex set of } R^{n1},$$

$$Y = \text{a closed convex set of } R^{n2},$$

$$f(\cdot), F(\cdot): X \times Y \rightarrow R^{1}.$$

$$g(\cdot): X \times Y \rightarrow R^{m}.$$

Using this notation, the bi-level programming problem is formulated as:

$$P1 \quad \max F(x, y) \tag{1}$$

where y solves

$$\max_{y} \quad f(x, y) \tag{2}$$

s.t.
$$g(x, y) \leq 0$$
 (3)

$$x \in X, \quad y \in Y \,. \tag{4}$$

For problem P1, the following definitions are needed:

DEFINITION 1. For $x \in X$, the set $\overline{S}(x) = \{y : y \in Y, g(x, y) \le 0\}$ is called the follower's solution set.

DEFINITION 2. For $x \in X$, the set $RR(x) = \{y \in \arg \max f(x, y) : y \in \overline{S}(x)\}$ is called the follower's rational reaction set.

The rational reaction set of the follower may be empty and may not be a singleton. In order to avoid this difficulty, for the purposes of Section 2-4 we will assume that:

[A1] if x^* is an optimal solution for the leader, then $RR(x^*)$ is a singleton.

DEFINITION 3. The feasibility set of problem P1 is denoted by:

$$S = \{(x, y) \colon x \in X, y \in RR(x)\}.$$

Problem P1 can be rewritten using this notation as:

$$P2 \max_{x,y} F(x,y) \tag{5}$$

s.t.
$$(x, y) \in S$$
. (6)

In the case where all functions are linear, the problem becomes a bi-level linear program which is formulated as follows:

$$P3 \max F(x, y) = ax + by \tag{7}$$

where y solves

$$\max_{y} \quad f(x, y) = cx + dy \tag{8}$$

s.t.
$$g(x, y) = Ax + By - p \le 0$$
 (9)

$$x, y \ge 0. \tag{10}$$

For problem P3 we have $X = R_{+}^{n1}$, $Y = R_{+}^{n2}$.

Once x is given, the follower's objective function is simply dy, and cx can be dropped from (8).

3. A Penalty Function Approach

3.1. THEORETICAL RESULTS

The proposed approach for solving bi-level linear programming is now developed. It involves the use of the fact that a duality gap for the follower is zero, for any specific $x \in X$, such that $\overline{S}(x) \neq \phi$ (see Section 6.1 for related work of Bard [6]).

For the linear program given by P3, where the follower's primal problem is given by (8)-(10), for a given x, ignoring the constant term cx, the follower's dual problem is:

$$P4 \min_{w} w(p - Ax) \tag{11}$$

s.t.
$$wB \ge d$$
 (12)

$$w \ge 0. \tag{13}$$

Given x and some values of w and y that satisfy the dual and primal constraints of the follower's problem, the optimal value of the follower's objective function lies in the interval [cx + dy, cx + w(p - Ax)]. When the duality gap, given by $\pi(x, y, w) = [w(p - Ax) - dy]$, is equal to zero, then the follower's optimal solution, for the given x, would be reached. Thus, it is possible to formulate the overall problem P3 as (see Theorem 3 later):

P5
$$P(K) = \max_{x, y, w} \hat{F}(x, y, w, K) = (ax + by) - K(w(p - Ax) - dy)$$
 (14)

s.t.
$$Ax + By \leq p$$
 (15)

$$wB \ge d \tag{16}$$

$$x, y, w \ge 0 \tag{17}$$

where $K \in R_+$.

DEFINITION 4. (i) The feasible region of w is given by

$$W = \{w: wB \ge d, w \ge 0\}.$$

$$(18)$$

(ii) The *feasible region of* z = (x, y) is given by

$$Z = \{(x, y) : Ax + By \le p, x \ge 0, y \ge 0\}.$$
(19)

(iii) The extreme points of W and Z are denoted by W_v and Z_v respectively.

It will be assumed that:

[A2] W and Z are non-empty bounded polyhedra, i.e. polytopes.

In the following, Theorems 1–4 are to be found in Anandalingam and White [4].

THEOREM 1. For a given value of $w \in W$ and fixed $K \in R_+$, define:

$$\Theta(w, K) = \max_{x, y} \left[\hat{F}(x, y, w, K) \colon (x, y) \in Z \right].$$
(20)

Then $\Theta(\cdot, K)$ is convex on \mathbb{R}^m (see [20], Theorem 5.5), and a solution to the problem:

$$\max\left[\Theta(w, K) \colon w \in W\right] \tag{21}$$

will occur at some $w^* \in W_v$ (see [8], Theorem 3.46).

THEOREM 2. For fixed $K \in R_+$, an optimal solution to problem P5 is achievable in $Z_v \times W_v$, and $Z_v \times W_v = (Z \times W)_v$.

THEOREM 3. There exists a finite value, $K^* \in R_+$, of K for which an optimal solution to the penalty function problem P5 yields an optimal solution to the problem P3, $\forall K \ge K^*$.

THEOREM 4. ([8], Lemma 9.2.1). If (x(K), y(K), w(K)) solves P(K) as a function of K, both the leader's objective F(x(K), y(K)) and the duality gap,

 $\pi(x(K), y(K), w(K))$, of the follower's rational reaction problem are monotonically non-increasing in the value of the penalty parameter K.

A special situation arises in Theorem 3 when b = d, i.e., the leader and follower are in unison over the choice of y given x. In this case, $K^* = 0$.

Theorem 2 gives us the essential features of an algorithm that could be used to provide a quasi-local optimum for the bi-level linear programming problem. For a given K, the first obvious step is to begin with an arbitrary (x^0, y^0) and solve the linear program $\{\max \hat{F}(x^0, y^0, w, K) : w \in W_v\}$ to obtain an optimal $w^0 =$ $w(x^0, y^0, K)$. Then with $w = w^0$, find $(x^1, y^1) \in \arg \max[\hat{F}(x, y, w^0, K) : (x, y) \in$ $Z_v]$. Then find $w^1 = w(x^1, y^1, K)$, and repeat. This will lead to a partial optimal solution for P(K). As Wendell and Hurter [25] have pointed out, in general, a partial optimal solution may not be locally optimal. However, because $\hat{F}(\cdot, \cdot, \cdot, K)$, is bi-linear, the type of problem that is being solved belongs to a class of problems for which Wendell and Hurter [25] show that a partial optimum for P(K) is locally optimal for P(K) as well. If K is large enough, this solution will be a local optimum for the bi-level linear program. It will be shown that the penalty function approach can be developed to find a global optimum.

Note that, although we have assumed that A1 and A2 hold, Theorems 1, 2, and 4 use A2 only and Theorem 3 uses A1 and A2. The development of a global optimization algorithm is now considered. This algorithm will begin with a large value of K, and increase it until the problem P3 is solved. If we find an appropriate K^* for Theorem 3, then we only need to use this one value of K^* . However, K^* may be very large, and lead to computational instabilities. It is, however, possible for the penalty contribution in P5 to become zero for a smaller value of K than any upper bound we may wish to use, in which case the solution obtained will solve problem P3 ([8], Theorem 9-2-1, Corollary). If we wish to use an upper bound, one is given by (45) in Section 6.1.

As pointed out in Section 1 there are other advantages in using a sequential K generation, related to the use of loss of optimality considerations studied in Section 5.

3.2. DEVELOPMENT OF THE ALGORITHM

Consider the problem P5. For a given K and w, let (x(w, K), y(w, K)) be a solution to (20). Some properties of the penalty function formulation of the problem described by P5, P(K) and $\Theta(\cdot, K)$ are now considered. Theorem 5 is given in Anandalingam and White [4].

THEOREM 5. For $u, w \in W$:

$$\Theta(u, K) \ge \Theta(w, K) - K(u - w)(p - Ax(w, K)).$$
⁽²²⁾

For given $u, w \in W$ and fixed $K \in R_+$, define

$$\Phi(u, w, K) = (u - w)(p - Ax(w, K)).$$

Then from Theorem 5, if $\Phi(u, w^1, K) < 0$, we have:

$$w^{1} \not\in \arg \max\{\Theta(w, K) \colon w \in W\}$$
. (23)

Expression (23) provides a mechanism for choosing the next vertex in any solution procedure for maximizing $\Theta(\cdot, K)$. Thus suppose that, at a particular iteration, w^1 is the current vertex. Using w^1 , we obtain $\Theta(w^1, K)$ and obtain an optimal solution $(x(w^1, K), y(w^1, K))$. The next step is to examine the adjacent vertices $\{w^{1s}\}$ of w^1 . If $\Theta(w^{1s}, K) > \Theta(w^1, K)$ for some s, select w^{1s} as the next vertex to go to and set $w^1 = w^{1s}$. Otherwise, check to see if $\Phi(w^*, w^1, K) < 0$ for some $w^*(w^1, K) \in W_n$. If so, select $w^*(w^1, K)$ as the next vertex to go to and set $w^1 = w^*(w^1, K)$. Repeat the procedure. If neither of the cases arise, then w^1 is a local optimum of $\Theta(\cdot, K)$ in W, and use will be made of part of Tuy's method (see [15] for details) to get the next local optimum. See Steps 5-10 below for details. Global optimality is reached at (x^*, y^*, w^*) when one can get the largest possible value of $\hat{F}(\cdot, \cdot, \cdot, K)$ and also satisfy the optimality conditions of the follower, i.e. if $\pi(x^*, y^*, w^*) = 0$, (x^*, y^*) will then solve P3. The zero duality gap is achieved monotonically (by Theorem 4) and at a finite K (by Theorem 3). Thus a procedure that will increase K in incremental steps, and obtain a global optimal solution of P(K) for each value of K, will yield a global optimal solution of the problem P3.

It is possible also to find a local optimal solution of the problem P3 by finding a local optimal solution $\hat{F}(\cdot, \cdot, \cdot, K)$ for each value of K, and increasing K in small increments until $\pi(x(K), y(K), w(K)) = 0$ where (x(K), y(K), w(K)) is local optimum.

Algorithm for Global Optimum

Step 0 Choose K (large) and $w^1 \in W_v$, $\Theta^1 = -\infty$, $\bar{w}^1 = w^1$.

Step 1 Find $\Theta(w^1, K)$. Obtain $(x(w^1, K), y(w^1, K))$, and set $\Theta^1 = \max[\Theta^1, \Theta(w^1, K)]$

$$\bar{w}^{1} = \begin{cases} w^{1} \text{ if } \Theta(w^{1}, K) > \Theta^{1} \\ \bar{w}^{1} \text{ if } \Theta(w^{1}, K) \leq \Theta^{1} \end{cases}.$$

Step 2 Let $\{w^{1s}\}$ be the adjacent vertices of w^1 , $1 \le s \le N(w^1)$. If $\Theta(w^{1s}, K) > \Theta^1$ for some s, set $w^1 = w^{1s}$ and $\Theta^1 = \Theta(w^1, K)$. Go to Step 2 Step 3 If $\Theta(w^{1s}, K) \leq \Theta^1, \forall s$, Find $\Gamma(w^1, K) = \min[(\Phi w, w^1, K): w \in W].$ Obtain $w^*(w^1, K)$. Step 4 If $\Gamma(w^1, K) < 0$ then set $w^1 = w^*(w^1, K)$. Go to Step 1. Step 5 If $\Gamma(w^1, K) \ge 0$ extend unit rays $\{t^{1s}\}$ along the edges from w^1 , and find $\alpha_s = \max[\alpha \ge 0: \Theta(w^1 + \alpha t^{1s}, K) \le \Theta^1], \ 1 \le s \le N(w^1).$ Step 6 Let $v^{1s} = w^1 + \alpha_s t^{1s}, 1 \le s \le N(w^1)$, $\wedge (w^1) = \{ \lambda = (\mu, \sigma) \in \mathbb{R}^{m+1} :$ $\mu w^{1} - \sigma \leq 0, \ \mu v^{1s} - \sigma \geq 0, \ 1 \leq s \leq N(w^{1}), \ \sigma \in [1, -1]\},$ and, for $w \in W$: $G(w, w^{1}) = \min[\mu w - \sigma; \lambda \in \wedge(w^{1})].$ Step 7 Let $w^{1*} \in \arg \max[G(w, w^1); w \in W]$. Step 8 If $G(w^{1*}, w^1) \le 0$ then $\bar{w}^1 \in \arg \max[\Theta(w, K) : w \in W]$, and the optimal value of $\Theta(\cdot, K)$ is reached for the particular K, with the solution $(x(\bar{w}^1, K), y(\bar{w}^1, K))$ (see Section 3.3(b)). Go to step 10. Step 9 If $G(w^{1*}, w^1) > 0$, set $w^1 = w^{1*}$.

Go to step 1 (see Section 3.3(c)).

Step 10 If $\pi(\bar{x}(w^1), \bar{y}(w^1), \bar{w}^1 > 0)$, set $K = K + \Delta$. Go to step 1. Otherwise $\pi(\bar{x}(w^1), \bar{y}(w^1), \bar{w}^1) = 0$ and, $(x(\bar{w}^1), y(\bar{w}^1))$ solves P3.

Obtaining adjacent vertices in Step 2 is quite simple; we use the concept that an extreme vector in a polytope is made up to basic and nonbasic variables. Some bookkeeping is required within Step 2 to make sure that each adjacent vertex examined is different from the previous one. However, when one leaves Step 2, only the current vertex needs to be stored and carried forward.

Steps 5–8 are modifications of the original algorithm proposed by Tuy [24]. It involves generating cones at local optimal solutions (Step 5), making sure that the generated cone includes the feasible region (Steps 6–7), and testing to see if a vertex included in the cone is better than the local optimal solution for the current value of K (Step 8). Horst and Tuy [17] provide a detailed description, both verbal and mathematical, of these kinds of cone splitting algorithms (page 195 ff). Each time the algorithm passes through Steps 5–8, the size of the feasible region that is under examination reduces. Steps 5–8 involve procedures for adding cones which requires further bookkeeping.

3.3. SOME ALGORITHMIC AND OPTIMALITY CONSIDERATIONS

(a) Correlated Objectives

The choice of w^1 in Step 0 is arbitrary. However, if b and d are close to each other the following selection procedure might be helpful.

- (i) Select $(\bar{x}, \bar{y}) \in \arg \max[ax + dy: (x, y) \in Z]$.
- (ii) Select $w^1(K) \in \arg \max[\hat{F}(\bar{x}, \bar{y}, w, K) : w \in W]$.

We will have $(\bar{x}, \bar{y}) \in S$. The following result shows how good such a procedure may be:

THEOREM 6. For all $K \ge 0$:

$$\Theta(w^{1}(K), K) \ge \max[\Theta(w, K): w \in W]$$

+ min[(b - d)y: (x, y) \in Z] - max[(b - d)y: (x, y) \in Z].

Proof. See Appendix.

If b and d are almost negatively correlated, then the following modification of (i) above might be helpful.

(i) Select $(\bar{x}, \bar{y}) \in \arg \max_x \min_y [ax - dy : (x, y) \in Z]$.

We will have $(\bar{x}, \bar{y}) \in S$.

We then have the following supporting result.

THEOREM 7. For all K > 1:

$$\Theta(w^{1}(K), K) \ge \max[\Theta(w, K): w \in W]$$

+ min[(b + d)y: (x, y) \in Z] - max[(b + d)y: (x, y) \in Z].

Proof. See Appendix.

Finally, it is of interest to see how good the solutions (\bar{x}, \bar{y}) , given in Theorems 6 and 7, are for the leader. We have the following theorem.

THEOREM 8. Let (\bar{x}^r, \bar{y}^r) be the solutions selected in steps (i) with r = 1, 2, respectively in Theorems 6 and 7, and (x^*, y^*) be an optimal solution to P3. Then:

(i)
$$F(x^*, y^*) \ge F(\bar{x}^1, \bar{y}^1) \ge F(x^*, y^*) + \min[(b-d)y : (x, y) \in Z]$$

 $-\max[(b-d)y : (x, y) \in Z].$ (24)

(ii)
$$F(x^*, y^*) \ge F(\bar{x}^2, \bar{y}^2) \ge F(x^*, y^*) + \min[(b+d)y: (x, y) \in Z]$$

 $-\max[(b+d)y: (x, y) \in Z].$ (25)

Proof. See Appendix.

(b) Degeneracy

If W is degenerate, then in Step 2 the adjacent vertices may have the same value of w^1 . The algorithm then skips all the way to Step 5 and proceeds from there.

If W is non-degenerate, then in Step 6, $\wedge(w^1)$ may be replaced by the singleton:

$$\wedge (w^{1}) = \{ \lambda = (\mu, \sigma) \in \mathbb{R}^{m+1} : w^{1}\mu - \sigma \le 0, v^{1s}\mu - \sigma = 0, \\ 1 \le s \le N(w^{1}), \sigma \in [1, -1] \}.$$

In both this case, and in the degenerate case, the optimality of $\Theta(\bar{w}^1, K)$ in Step 8 follows because, under the circumstances postulated, we must have

 $W \subseteq \text{convex hull } \{w^1, \{v^{1s}\}\},\$

and then, using the convexity of $\Theta(\cdot, K)$, w^1 is optimal.

Step 3 is a standard linear program.

In the general case, Steps 7 and 8 may be executed by linear programming. Let

 $\{\lambda^1\}, 1 \le t \le T(w^1)$ be the vertices of $\wedge(w^1)$. Then the primal linear program is as follows.

L.P.
$$(w^{1})$$
 max $[\Psi]$
s.t. $\Psi - w\mu^{t} \leq -\sigma^{t}$, $1 \leq t \leq T(w^{1})$
 $-wB \leq -d$
 $w \geq 0$.

The vertex set $\{\lambda^i\}$ will not, in general be known explicitly. To overcome this difficulty we use the dual of L.P. (w^1) and the column generation method of Dantzig and Wolfe [12]. The dual linear program is as follows, where σ is the vector with components $\{\sigma^i\}$ and μ is the matrix with columns $\{\mu^i\}$.

D.L.P.(w¹) min[
$$\tau = -\sigma\beta - d\gamma$$
]
s.t. $\sum_{t=1}^{T(w^1)} \beta_t = 1$
 $-\mu\beta - B'\gamma \ge 0$,
 $\beta \ge 0, \gamma \ge 0$.

If δ is the current simplex multiplier for the first constraint and ξ is the current simplex multiplier vector for the second set of constraints, then, at the current solution to D.L.P(w^1), the shadow cost of β_t is:

$$\xi\mu^t-\sigma^t-\delta$$
.

The candidacy of any β_i as a potential basic variable arises only if

$$(\mu^{t}, \sigma^{t}) = \lambda \in \arg\min_{\lambda \in \wedge(w^{1})} [\xi \mu - \sigma - \delta]$$

and

$$\min_{\lambda \in \wedge (w^1)} \left[\xi \mu - \sigma - \delta \right] \leq 0.$$

Thus, we do not need to list $\{\lambda^t\}$ in advance.

The candidacy of any component of γ as a potential basic variable is a straightforward matter. Once the dual problem D.L.P.(w^1) has been solved, if $\tau \leq 0$, we have $\Psi \leq 0$ and termination occurs at Step 8. If $\tau > 0$, then $\Psi > 0$ and we use the dual solution to generate w^{1*} for Step 9.

(c) Cycling

This process must terminate in a finite number of steps unless there is cycling. Cycling occurs if, at iteration r, the best solution, $w_r^{1^*}$, obtained at Step 9, is the same as w_q^1 for some q < r. In order to avoid this, we do the following:

Let S_v be the set of vertices at W that are fathomed using Steps 2, 4, and 5 above. Let A_v be the set of vertices of W which are adjacent to some $w \in S_v$. If $A_v \backslash S_v = \emptyset$, then $S_v = W_v$, and the process terminates with an optimal solution. If cycling occurs at iteration r, and $A_v \backslash S_v \neq \emptyset$, then select any $w \in A_v \backslash S_v$, instead of w_r^{1*} . Since the set W_v is edge connected, the process will terminate in a finite number of steps.

4. Computational Results

Table I provides the results of a computational exercise of running 50 randomly selected problems of 6 different sizes for each method. The size of the problem is denoted by (n_1, n_2, m) where n_1 and n_2 stand for the dimension of the leader's and follower's decision vectors respectively, and m is the number of constraints. All problems were run on an ATT PC6300+ microcomputer with Intel 80286 microprocessor, and 80287 math co-processor. The linear programs in the penalty function or the k-th best algorithms were solved using the LINDO package, and pascal programs linked the different components of the iteration together. The Bard and Moore [7] branch-and-bound method was implemented by modifying the code sent by Bard, which uses XMP for the linear programming part.

The characterization of the problems generated was completely random; i.e. the coefficients of the problems were generated from a uniform distribution. The objective function parameters were all generated randomly to be in the closed set (-10, +10). No attempt was made to check if the values of b and d were the same or close. The constraint parameters were generated randomly in the closed set (-5, +5). We varied the matrix density from 10% of non-zero terms to 75%. We did not identify which of these problems took the longest to solve or which ones produced degenerate solutions.

The first test was to ensure that the problems were feasible from the point-ofview of the leader. Infeasible problems were discarded, and not included in the final results. It should be noted that around 50% of the randomly generated problems were discarded because of infeasibility. Clearly, if the values of b and d are close [see (7)-(10)], the corresponding bi-level program would be easier to solve. However, we recorded average run times for problems that were solved, and did not flag cases that were solved more easily than others.

F (·F = ·······	
Problem size	k-th Best time	Branch-and-Bound time	Penalty Method time
(5, 10, 6)	127.6	55.2	59.3
(6, 14, 8)	111.7	81.9	87.2
(8, 17, 10)	186.2	102.1	102.7
(15, 30, 20)	1200.9	151.7	167.8
(50, 50, 100)	_	1043.9	1821.3

Table I. Algorithmic performance (time = cpu seconds)

The penalty function method involves the setting up of a large value of the penalty parameter K, especially because we have proved that there is an exact value (Theorem 3). The starting value of K is chosen through experimentation. First, a very large value of K (say 1000) and a reasonable value (say 10) are chosen in turn. If the final results are very different, then K is set at 10 and at each Step 10, K is increased by $\Delta = 1$ (i.e. a 10% increase), until optimality is changed. If the final results for K = 10 and K = 1000 are the same, these results are taken as optimal. This test involves an extra step and additional computation time associated with that step. However, the test reduces the average time of the computations. The choice of Δ also influences the computation time, but we have not evaluated its impact.

We compared the penalty method proposed in this paper with the Bard-and-Moore [7] branch-and-bound method and with the Bialas and Karwan's [10] k-th best method. The penalty function method proposed in this paper does worse than Bard's [6] branch-and-bound method in terms of cpu time, but easily outperformed the k-th best method. The time taken by the penalty function is comparable to the branch-and-bound method for problems of small size, but the branch-and-bound method does better for larger problems.

5. Relationship of the Penalty Function Approach to the Leader-Follower Game

For a given value of K, an optimal solution (x(K), y(K)) to P5 will not, in general, give a leader-follower solution to the noncooperative game; i.e. in general $y(K) \not\in RR(x(K))$. This is because y(K) is a component of the maximand of the hybrid objective $\hat{F}(\cdot, \cdot, \cdot, K)$ for a particular value of K, and not necessarily the follower's reaction to x(K). However, for any particular value of K for which the duality gap, $\pi(x(K), y(K), w(K))$, becomes zero, $y(K) \in RR(x(K))$.

Suppose that, for x = x(K), the follower solves his problem and gets $\tilde{y}(K) \in RR(x(K))$. Since the proposed penalty function approach results in y = y(K), instead of the rational reaction $\tilde{y}(K)$, then it is of interest to compute the follower's loss of optimality if y(K) is used instead of $\tilde{y}(K)$. At any value of K, if $\tilde{w}(K)$ is an optimal dual solution for the follower, associated with $\tilde{y}(K)$, then:

$$\pi(x(K), y(K), w(K)) = w(K)(p - Ax(K)) - dy(K), \qquad (26)$$

and

$$\pi(x(K), \, \tilde{y}(K), \, \tilde{w}(K)) = \tilde{w}(K)(p - Ax(K)) - d\tilde{y}(K) = 0 \,, \tag{27}$$

where the last equality follows since, for a given x(K), $(\tilde{y}(K), \tilde{w}(K))$ is an optimal solution to the follower's problem, and thus the duality gap is zero. From (26) and (27) it follows that:

$$d\tilde{y}(K) - dy(K) = (\tilde{w}(K) - w(K))(p - Ax(K)) + \pi(x(K), y(K), w(K)).$$
(28)

 $w = \tilde{w}(K)$ is an optimal dual solution for the follower's problem, and the first term on the right-hand-side of (28) is non-positive. Thus, if the follower's loss, that results from playing y(K) instead of $\tilde{y}(K)$, is defined by:

$$F.L(K) = d\tilde{y}(K) - dy(K)$$
⁽²⁹⁾

then

$$0 \le F.L.(K) \le \pi(x(K), y(K), w(K)).$$
(30)

This gives an upper bound on the follower's loss.

Finally, consider the situation where the follower insists on playing $\tilde{y}(K)$ at each iteration when the leader plays x(K). In this case if (x^*, y^*) solves P3, to determine the leader's loss of optimality we have to establish bounds for the difference:

$$L.L(K) = ax^* + by^* - ax(K) - b\tilde{y}(K) \ge 0.$$
(31)

The inequality (31) follows because, at any iteration K, $(x(K), \tilde{y}(K))$ is in the feasibility set S, and (x^*, y^*) is optimal in S for the leader. We easily obtain

$$ax^{*} + by^{*} - ax(K) - b\tilde{y}(K) \leq b(y(K) - \tilde{y}(K)) - K\pi(x(K), y(K), w(K)).$$
(32)

Thus an upper bound on the loss of optimality for the leader if he uses x = x(K)and the follower uses $y = \tilde{y}(K)$ is given by:

$$L.L(K) \le b(y(K) - \tilde{y}(K)) - K\pi(x(K), y(K), w(K)).$$
(33)

In (33), $K\pi(x(K), y(K), w(K)) \rightarrow 0$ as $K \rightarrow K^*$. Also, for $K \ge K^*$, as a result of assumption A1, $y(K) = \bar{y}(K)$.

The use of the above results depends upon the circumstances surrounding the actual resolution of the problem P3. We consider some possibilities.

(a) If the penalty model is used by the leader to determine x(K), without knowing x^* , and the follower always chooses $\tilde{y}(K)$, then (33) gives an upper bound on the loss of optimality for the leader, enabling him to decide whether or not to seek a better solution.

If $\tilde{y}(K)$ is not uniquely determined for the follower, then the best upper bound for the loss of optimality for the leader, on the basis of the above information, is given by:

$$L.L(K) \leq \max_{\tilde{y} \in RR(x(K))} \left[b(y(K) - \tilde{y}) \right] - K\pi(x(K), y(K), w(K)) .$$
(34)

If $\{x(K), y(K), w(K)\}$ are not uniquely determined, then if, for a specified value of K, U(K) is the set of optimal $\{x(K), y(K), w(K)\}$ solutions, (34) can be replaced by:

$$L.L(K) \le \min_{(x,y,w) \in U(K), \ \bar{y} \in RR(x)} \max_{[b(y-\bar{y}) - K\pi(x, y, w)]} .$$
(35)

(b) If both the leader and the follower agree to use the solutions to the penalty model, and if w^* is an optimal dual solution, given x^* , the leader's gain, over $ax^* + by^*$, is

$$L.G(K) = ax(K) + by(K) - ax^* - by^*$$

= $\hat{F}(x(K), y(K), w(K), K) + K\pi(x(K), y(K), w(K))$
- $\hat{F}(x^*, y^*, w^*, K) - K\pi(x^*, y^*, w^*)$. (36)

Now

$$\hat{F}(x(K), y(K), w(K), K) \ge \hat{F}(x^*, y^*, w^*, K)$$
(37)

and

$$\pi(x^*, y^*, w^*) = 0.$$
(38)

Hence the gain for the leader satisfies:

$$L.G(K) \ge K\pi(x(K), y(K), w(K)).$$
⁽³⁹⁾

It is seen that the lower bound in (39) in K times the upper bound (30). This may give some scope to allow the leader to pay the follower to adopt an (x(K), y(K)) solution. If (x(K), y(K), w(K)) is not uniquely determined, then the appropriate (x(K), y(K)) solution, with compensation to the follower, may be sought.

(c) The leader may use the solution to the penalty problem and the follower may use a rational reaction solution, as in (a), but when the rational reaction solution set is not a singleton, the follower may be induced, by a payment, to choose the one which minimizes, rather than maximizes, the upper bound on the loss of optimality for the leader. Thus "max" is replaced by "min" in (34). In this case, the known loss of optimality, given x(K), for the follower is zero.

6. Linear and Nonlinear Duality Formats

6.1. THE LINEAR DUALITY FORMAT OF BARD [6]

For the problem P3 an alternative version of penalty problem P5 is:

$$Q5 \quad Q(K) = \max_{x, y, w} \left[\hat{G}(x, y, w, K) = ax + by - K(w(p - Ax - By)) \right]$$
(40)

subject to constraints (15)–(17). Bard [6] uses this penalty function approach for levels 2 and 3 of a 3 level problem, not to solve the levels 2 and 3 problem, but essentially, via his Theorem 2, to provide an upper bound for the level 1 objective function value. Step 2 of Bard's three level problem for solving the problem at levels 2 and 3, uses an unspecified algorithm. If, however, we fix the level 1 decision vector, x^1 , at 0, the levels 2 and 3 problem reduces to a two level problem for which the penalty form Q(K) might be used in a similar manner.

The analysis for Q(K) follows in exactly the same manner as for P(K). The difference between P(K) and Q(K) is that P(K) uses the duality gap as the penalty contribution, and Q(K) uses the complementary slackness function as the penalty contribution. There is some advantage in using P(K) rather than Q(K). It is easily seen that, for all feasible, x, y, w, and $K \in R_+$:

$$\hat{G}(x, y, w, K) = \hat{F}(x, y, w, K) + K(wB - d)y.$$
(41)

In view of constraints (16), (17), we have:

$$\hat{G}(x, y, w, K) \ge \hat{F}(x, y, w, K), \qquad (42)$$

and

$$Q(K) \ge P(K) , \quad \forall K \in R_+ .$$
⁽⁴³⁾

Now both $\{Q(K)\}$ and $\{P(K)\}$ converge, non-increasing, to the optimal value of the leader's objective function as $K \rightarrow \infty$. Thus, for any given $K \ge 0$, P(K) provides at least as good an upper bound as does Q(K). Also $\{P(K)\}$ may converge more quickly.

A key question is: how big should K be in order to guarantee that solving the penalty problems P5 and Q5 will solve the bi-level problem, bearing in mind the possibility that solutions may be obtained before we reach any specific upperbound on K needed for this guarantee? A priori bounds, used to establish Theorem 3 are, respectively:

$$K(Q) = \max[(ax + by - a\hat{x} - b\hat{y})/w(p - A\hat{x} - B\hat{y})]$$

(x, y) $\in Z_v$, (\hat{x}, \hat{y}) $\in Z_v$
 $w(p - A\hat{x} - B\hat{y}) > 0$, $w \in W_v$, (44)

$$K(P) = \max[(ax + by - a\hat{x} - b\hat{y})/(w(p - A\hat{x}) - d\hat{y})]$$

(x, y) $\in Z_v$, $(\hat{x}, \hat{y}) \in Z_v$
 $w(p - A\hat{x}) - d\hat{y} > 0$, $w \in W_v$. (45)

Given the constraints (15)-(17) we see that

$$K(Q) \ge K(P) . \tag{46}$$

6.2. NONLINEAR DUALITY FORMAT

For non-linear problems of the general kind P1, it is possible to generalize P5. We will assume that appropriate conditions hold for the strong duality results to hold (e.g., see [14], Theorem 3). Then the dual function for the follower's problem, given $x \in X$ is, with $w \in \mathbb{R}_+^m$:

$$h(x, w) = \max_{v \in Y} \left[f(x, v) - wg(x, v) \right].$$
(47)

The analogue of P5 then becomes:

$$P6 \quad \tilde{P}(K) = \max_{x, y, w} \left[\tilde{F}(x, y, w, K) = F(x, y) - K(h(x, w) - f(x, y)) \right]$$
(48)

s.t.
$$g(x, y) \leq 0$$
 (49)

$$x \in X, \quad y \in Y, \quad w \in \mathbb{R}^m_+. \tag{50}$$

In the linear case, this reduces to P5. It is to be noted that, although the complementary slackness conditions

$$wg(x,v) = 0 \tag{51}$$

hold in (47), at an optimal solution to (48), we have no analogue of (16) in the general non-linear case, and hence it is not possible to produce an analogue of Bard's Q5 formulation. Given the strong duality conditions problem P6 takes the form:

$$P7 \quad \tilde{P}(K) = \max_{x, y, w} \min_{v} \left[F(x, y) + Kf(x, y) - K(f(x, v) - wg(x, v)) \right]$$
$$= \min_{v} \max_{x, y, w} \left[F(x, y) + Kf(x, y) - K(f(x, v) - wg(x, v)) \right]$$
s.t. $x \in X$, $y \in Y$, $w \in R_{+}^{m}$, $v \in Y$.

For the linear problem, with $X = R_{+}^{n1}$, $Y = R_{+}^{n2}$, problem P7 takes the form, alternatively to problem P5:

$$P8 \quad \tilde{P}(K) = \max_{x, y, w} \min_{v} [ax + by + Kd(y - v)]$$
$$= \min_{v} \max_{x, y, w} [ax + by + Kw(Ax + Bv - p)]$$
s.t. $x \in R_{+}^{n1}, y \in R_{+}^{n2}, w \in R_{+}^{m}, v \in R_{+}^{n2}$

The theoretical analysis for the general non-linear case, subject to the strong duality requirement, is much more difficult than for the linear case. Nonetheless the above format does provide a framework for tackling this problem.

If $\Theta(\cdot, K)$ is defined analogously to (20), then Theorem 1 will not hold in

general. Indeed, without the reduction possible for the linear form in (14)–(17), $\Theta(\cdot, K)$ is neither convex nor concave in general. Finding algorithms for problem P7 is a challenge. Problem P8 is a bi-linear, max min problem which provides a challenge for the extensions of ordinary bi-linear programming.

If we define a function $\Gamma(\cdot, K)$ on \mathbb{R}^{n^2} by:

$$\Gamma(v, K) = \sup_{x, y, w} [F(x, y) + Kf(x, y) - K(f(x, v) - wg(x, v))]$$

s.t. $x \in R_+^{n1}$, ycR_+^{n2} , $w \in R_+^m$,

then problem P7 takes the form:

P9
$$\tilde{P}(K) = \min_{v} [\Gamma(v, K)]$$

s.t. $v \in \mathbb{R}^{n^2}_+$.

This is a convex, non-differentiable, optimization problem for which techniques exist. For problem P6 we have the following results:

- (i) Theorem 2 will not hold in general.
- (ii) If A1 holds and the feasible regions are non-empty, convex and compact, then Theorem 3 will be replaced by an appropriate convergence result, with no finite exact penalty parameter value existing in general. Thus, in this case the sequential K analysis is important.
- (iii) Theorem 4 will hold for non-empty compact feasible regions.
- (iv) Theorem 5 will not hold, but it may be possible to produce a corresponding result to assist any algorithm.
- (v) Theorems 6, 7, 8 will need revising in some suitable form.

With the appropriate determination of duality gap, $\pi(x, y, w) = h(x, w) - f(x, y)$, then both (30) and (39) will hold. This thus allows us to use much the same requirements as given in Section 5, using the K-analysis to reach acceptable solutions. Also, as a consequence when $\pi(x(K), y(K), w(K)) = 0$, (x(K), y(K)) is an optimal solution.

The bounds on loss of optimality given in (33), (34) will need revision.

6.3. ASSUMPTION A1

Finally for P1, condition A1 may be relaxed by using the following, more general problem format PG1:

$$PG1 \max_{x} \min_{y} [F(x, y)]$$
(52)

s.t.
$$(2)-(4)$$
. (53)

$$PG5 \quad PG(K) = \max_{x,w} \min_{y} \left[\hat{F}(x, y, w, K) \right]$$
(54)

s.t. (15)–(17).

Problem formulation PG1 is already known.

For the problems PG1 and PG5, Theorem 4 will hold, and so will Theorem 3, without the requirement of assumption A1.

7. Summary and Comments

This paper develops a duality gap-penalty function format approach to the bi-level programming problem, which is applicable, in principle, to multi-decisionmaking, multi-level, non-linear problems. The duality gap-penalty function approach seems to be a natural way of capturing optimality characteristics, and of exploring the actual resolution of the decisionmaking process, as described in Section 5. The particular case of the linear problem is studied in detail, and an algorithm developed, using a modification of the method of Tuy to solve the nonconvex optimization problem derived. The computational results show that this particular nonconvex optimization approach is not as good as the Bard-Moore [7] branch-and-bound method, but is somewhat better than the k-th best method of Bialas and Karwan [10]. Thus, in its current form, it is non-competitive. However, supplemented by results shows those given in Theorems 6–8, the same format, but with a different optimizing algorithm, may perform better. The various bounding results have not been used in a branch and bound mode, but this is possible.

The results of Section 5 enable an interactive decisionmaking process to be developed in which the various solutions developed, coupled with associated bounds on loss of optimality, may be used to explore possible compromises.

In Section 6.1 arguments are given for some advantages of the proposed duality approach over that of Bard [6], in terms of the penalty parameter K. A theoretical framework for finding the critical K^* is also given, although we have not tackled the computational problem involved.

A format is given in Section 6.2 for the nonlinear problem, applicable to the earlier linear models. The computational problem is a challenging one, aided by any mathematical properties it is possible to develop. In general, it is not possible to produce an analogue of Bard's [6] approach. The non-linear penalty problem P6 leads to a min max bi-linear optimization problem in the linear case which provides a challenge for developing extensions of the standard bi-linear algorithms. In the non-linear case, the problem is reversible to a convex non-differentiable optimization problem, for which techniques exist. Finally we note that the singleton assumption A1 is weaker than the usual one required for other algorithms. It is not required at any stage of the computations except at a terminal point which is optimal and is only required for the derivation of the exact penalty function result.

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Appendix. Proof of Theorems

Proof of Theorem 6.

$$\Theta(w^{1}, K) = \max[ax + by - K(w^{1}(K)(p - Ax) - dy): (x, y) \in Z]$$

$$\geq \max[ax + dy - K(w^{1}(K)(p - Ax) - dy): (x, y) \in Z]$$

$$+ \min[(b - d)y: (x, y) \in Z]$$

$$\geq a\bar{x} + d\bar{y} - K(w^{1}(K)(p - A\bar{x}) - d\bar{y})$$

$$+ \min[(b - d)y: (x, y) \in Z]$$

$$= \max[ax + dy: (x, y) \in S]$$

$$+ \min[(b - d)y: (x, y) \in Z]$$

$$= \max[ax + dy - K(w(p - Ax) - dy): (x, y, w) \in Z \times W]$$

$$+ \min[(b - d)y: (x, y) \in Z]$$

$$\geq \max[ax + by - K(w(p - Ax) - dy): (x, y, w) \in Z \times W]$$

$$+ \min[(b - d)y: (x, y) \in Z] + \min[(d - b)y: (x, y) \in Z]$$

$$= \max[\Theta(w, K): w \in W]$$

$$+ \min[(b - d)y: (x, y) \in Z] - \max[(b - d)y: (x, y) \in Z]$$

Proof of Theorem 7.

$$\begin{split} \Theta(w^{1}, K) &= \max[ax + by - K(w^{1}(K)(p - Ax) - dy): (x, y) \in Z] \\ &\geq \max[ax - dy - K(w^{1}(K)(p - Ax) - dy): (x, y) \in Z] \\ &+ \min[(b + d)y: (x, y) \in Z] \\ &\geq a\bar{x} + (K - 1)d\bar{y} - K(w^{1}(K)(p - A\bar{x})) \\ &+ \min[(b + d)y: (x, y) \in Z] \\ &= \max[ax - dy: (x, y) \in S] \end{split}$$

Proof of Theorem 8.

(i) Using the optimality of (x^*, y^*) , and noting that $(x^*, y^*) \in S$, $(\bar{x}^1, \bar{y}^1) \in S$, we have:

$$F(x^*, y^*) \ge F(\bar{x}^1, \bar{y}^1) = a\bar{x}^1 + b\bar{y}^1$$

= $a\bar{x}^1 + d\bar{y}^1 + (b - d)\bar{y}^1$
 $\ge ax^* + dy^* + (b - d)\bar{y}^1$
= $ax^* + by^* + (b - d)\bar{y}^1 - (b - d)y^*$
 $\ge F(x^*, y^*) + \min[(b - d)y : (x, y) \in Z]$
 $- \max[(b - d)y : (x, y) \in Z]$.

(ii) Using the optimality of (x^*, y^*) and noting that $(x^*, y^*) \in S$, $(\bar{x}^2, \bar{y}^2) \in S$, we have:

$$F(x^*, y^*) \ge F(\bar{x}^2, \bar{y}^2) = a\bar{x}^2 + b\bar{b}^2$$

= $a\bar{x}^2 - d\bar{y}^2 + (b+d)\bar{y}^2$
 $\ge ax^* - dy^* + (b+d)\bar{y}^2$
= $ax^* + by^* + (b+d)\bar{y}^2 - (b+d)y^*$
 $\ge F(x^*, y^*) + \min[(b+d)y : (x, y) \in Z]$
 $- \max[(b+d)y : (x, y) \in Z].$

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