A Penalty-Function Approach to a Mixed-Integer Bilevel Programming Problem

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Abstract. In this paper, we present a mathematical framework for the problem of minimizing the cash-out penalties from the point of view of the natural gas shipper. The problem is modeled as a mixed bilevel linear programming problem. To solve it efficiently, we reformulate it as a standard mathematical programming problem and describe an algorithm of penalty functions for its solution. The algorithm is well-founded and its convergence is proved.

1 Introduction

In many decision processes there is a hierarchy of decision makers, and decisions are made at different levels in this hierarchy. One way to handle such hierarchies is to focus on one level and include other levels' behaviours as assumptions. Multilevel programming is the research area that focuses on the whole hierarchy structure. In terms of modeling, the constraint domain associated with a multilevel programming problem is implicitly determined by a series of optimization problems which must be solved in a predetermined sequence. If only two levels are considered, we have one leader (associated with the upper level) and one follower (associated with the lower one), and call the problem as a *bilevel programming problem*. If the constraints at both levels are all linear, we have a bilevel linear programming problem (BLP). In [1], one can find both the essencial fundamentals of the multilevel optimization and its applications to solution of real systems.

The field of multilevel optimization today is a well-known and important research field. Hierarchical structures can be found in diverse scientific disciplines including environmental studies, classification theory, databases, network design, transportation, game theory, and economics; and new applications (like the above described gas cash-out problem) are constantly being introduced. This is, in turn, positive for the development of new theory and efficient algorithms.

A particular case of the bilevel programming problem is presented by the following mixed-integer model arising from the problem of minimization of cash-out penalty costs of a natural gas shipping company. In countries like the United

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States, for instance, the natural gas industry has been going through a deregulation process since the mid-1980s leading to significant market changes. Now the decision making procedure of gas buying, selling, storing, transporting, etc., is immersed into a very complex world in which producers, pipelines (transporters), and brokers, all play quite important roles in the chain. This chain becomes even more complex if we take into account the network of pipelines transporting gas and oil throughout the Latin America, which reaches Canada at one edge and Argentina at the other edge, passing through the USA, Mexico, the Central and South Americas. In what concerns Mexico, it is very important to study and understand this complex phenomenon and moreover, to develop the supporting techniques that permits one to make decisions well-grounded when one needs to interact with the foreign counter-partners in the processes of buying/selling/transporting the gas.

The problem in question arises when a shipper draws a contract with a pipeline company to deliver a certain amount of gas among several points. What is actually delivered may be more or less of the amount that had been originally agreed upon (this phenomenon is called *an imbalance*). When an imbalance occurs, the pipeline penalizes the shipper by imposing a cash-out penalty policy. As this penalty is a function of the operating daily imbalances, an important problem for the shippers is how to carry out their daily imbalances so as to minimize their incurred penalty.

In [10], a mathematical framework for the above described problem is presented. The problem is modeled as a mixed-integer bilevel linear programming problem (BLP) where the shipper is the leader (upper level) and the pipeline represents the follower (lower level). Even the simplest version of a multilevel optimization problem, a linear problem with two levels, is known to be very hard to solve. Mixed-integer BLP possess even a higher degree of difficulty as the typical concepts for fathoming in traditional branch-and-bound algorithms for mixed-integer programming (MIP) cannot be directly applied to mixed-integer BLP. In order to find good solutions for this problem, the authors [10] propose a heuristic based on simulating annealing.

In this paper, our principal goal is to develop an efficient method for addressing the above-described problem of minimizing the cash-out penalties of the shipper (the leader) subject to the lower level problem reflecting the aims of the pipeline (the follower). We are going to consider a hierarchical system where a leader incorporates into its strategy the reaction of the follower to its decision. The follower's reaction is quite generally represented as the solution set to a monotone variational inequality (cf. [1], [2], [6]). For the solution of this nonconvex mathematical program a penalty approach will be applied, based on the formulation of the lower level variational inequality as a mathematical program. The algorithm is well-based and its convergence to a solution of the initial bilevel problem is established.

The paper is organized as follows. The problem is specified in Section 2, whereas the penalty function method is described in Section 3. The algorithm convergence results are also presented in Section 3, and Section 4 contains conclusions and directions of future research..

2 Problem Specification

First, we describe the problem in terms of [10], in order to illustrate the proposed methodology.

Assume that a shipper has entered into a contract (with other clients) to deliver a given amount of natural gas from a receipt to a delivery meter in a given time frame. (From now on, we treat "natural gas" and "gas" as synonims). The shipper must stipulate title transfer agreements with the meter operators and a transportation agreement with the pipeline. Under such agreements, the shipper nominates a daily amount of gas to be injected by the receipt meter operator into the pipeline and to be withdrawn by the delivery meter operator from the pipeline. The pipeline transports the gas from the receipt meter to the delivery meter.

Due to the nature of the natural gas industry, what is actually transported is inevitably different from what is nominated. Such a difference constitutes an imbalance. There exist operational and transportation imbalances. The first type of imbalance refers to differences between nominated and actual flows, while the latter involves differences between net receipts (receipts minus fuel) and deliveries. While pipelines allow for small imbalances, they issue penalties for higher (both operational and transportation) imbalances to the other parties. In the following, we assume that the shippers are held responsible for imbalance penalties, and we analyze the cash-out penalties associated with operational imbalances.

On the shipper side, an operational imbalance can be either positive or negative. A positive [negative] imbalance arises when the shipper leaves [takes] gas in [from] the pipeline. Alternatively, a positive [negative] imbalance means that the actual flow is smaller [greater] than the nominated amount of gas. A positive [negative] end-of-the-month imbalance implies as cash transaction from the pipeline [shipper] to the shipper [pipeline]. Cash-out prices are set in a way that whenever a shipper sells [buys] gas to [from] the pipeline, he does that at a very low [high] price. The relation between cash-out price and imbalance position depends non-linearly on the average, maximum and minimum gas spot price for the past month.

Shippers daily nominate gas flows taking into account the constraints deriving from their buy/sell activity, their contractual constraints, and future market opportunities. The gas price is one of the major factors affecting their decisions. In the absence of cash-out provisions, historically shippers would take out high cost gas in the winter from the pipeline (causing negative imbalances), and pay the transporter back with low cost gas in the summer. This corresponds to a speculative behaviour by the shippers, whereby imbalances are created and managed as pseudo-storage in order to take advantage of movements in the gas price. Cash-out penalties were designed in order to avoid such pricing arbitrages.

In the framework below, shippers are concerned with minimizing the cash-out penalties.

2.1 Notation

As stated in the previous subsection, the decision making process for the shipper (leader) is to determine how to carry out its daily imbalances so as to minimize the penalty that will be imposed by the pipeline (follower).

The following notation is used to describe the model.

Indices and Sets

i, j, k zone pool indices; $i, j, k \in J = \{1, 2, \dots, P\}$;

t time index; $t \in T = \{1, 2, \dots, N\}$.

Parameters

x_{ti}^L, x_{ti}^U bounds on daily imbalances at (end of) day t in zone i; $t \in T$, $i \in J$;

x_t^L, x_t^U bounds on total daily imbalances at (end of) day t; $t \in T$;

s_{ti}^L, s_{ti}^U bounds on balance swings during day t in zone i; $t \in T, i \in J$;

e_{ij} percentage of fuel retained for moving one dekatherm (dt) of gas from zone i to j; $i, j \in J$;

f_{ij} transportation charge for moving one dt of gas from zone i to j; $i, j \in J$, $i < j$;

b_{ij} backward haul credit for moving one dt of gas from zone j to i; $i, j \in J$, $i < j$;

x_{0j} initial imbalance (start of day 1) in zone j; $j \in J$.

Decision Variables

x_{ti} imbalance at (end of) day t in zone i; $t \in T$, $i \in J$;

s_{ti} imbalance swing during day t in zone i; $t \in T$, $i \in J$;

y_i final imbalance at zone i; $i \in J$;

u_{ij} forward haul volume moved from zone i to j; $i, j \in J$, $i < j$;

v_{ij} backward haul volume moved from zone j to i; $i, j \in J$, $i < j$;

z total cash-out revenue for shipper.

Auxiliary Variables

q binary variable equal to 1 (0) if final imbalances are nonnegative (non-positive).

2.2 Mathematical Model

Here we provide the set of constraints involved in both the upper and lower levels of the problem.

Upper Level Model:

Objective: Shipper's revenue.

$$\max h_1(x, s, y, u, v, z) = z, \tag{1}$$

subject to:

$$x_{ti}^L \le x_{ti} \le x_{ti}^U, \qquad t \in T,\ i \in J; \tag{2}$$

$$s_{ti}^L \le s_{ti} \le s_{ti}^U, \qquad t \in T,\ i \in J; \tag{3}$$

$$x_t^L \le \sum_{i \in J} x_{ti} \le x_t^U, \qquad t \in T; \tag{4}$$

$$x_{ti} = x_{t-1,i} + s_{ti}, \qquad t \in T, i \in J. \tag{5}$$

Lower Level Model:

Objective: The penalty is determined by minimizing the amount of cash transactions. In many cases, both shipper and pipeline agree in a policy that represents a compromise between them two, so rather that minimizing revenue for shipper, it is agreed to minimize deviations from zero. Hence, the following objective is given by

$$\min h_2(x, s, y, u, v, z) = |z|, \tag{6}$$

subject to the constraints below.

Balance constraints: This constraint identifies the relationship between the imbalance at day $N = |T|$, forward and backward haul volumes, retained fuel,and final imbalance at zone j:

$$y_j = x_{N,j} + \sum_{i:i<j} (1 - e_{ij}) u_{ij} + \sum_{k:k>j} v_{jk} - \sum_{k:k>j} u_{jk} - \sum_{i:i<j} v_{ij},\ j \in J; \tag{7}$$

Gas conservation: This constraint ensures no gas loss occurs. Although it follows directly from (7) after summation with respect to all $j \in J$, we keep it on to make the problem clearer to non-technical users.

$$\sum_{i \in J} y_i + \sum_{(i,j):i<j} e_{ij} u_{ij} = \sum_{i \in J} x_{N,i}. \tag{8}$$

Note that $\sum_{(ij)} e_{ij} u_{ij} \ge 0$, hence $\sum_i y_i \le \sum_i x_{N,i}$.

Zone upper bounds: This constraint prevents cyclic movements of gas. It simply states that, at any given zone, we cannot move more than any initial positive imbalance.

$$\sum_{i:i<j} u_{ij} + \sum_{k:k>j} v_{jk} \le \max\{0, x_{N,j}\}, \quad j \in J, \quad \text{such that } x_{N,j} > 0. \tag{9}$$

Forward haul upper bounds: These bounds prevent positive-to-positive and negative forward movement of imbalances.

$$u_{ij} \le \begin{cases} x_{N,i} & \text{if } x_{N,i} > 0 \text{ and } x_{N,j} < 0; \\ 0 & \text{otherwise.} \end{cases} \tag{10}$$

Backward haul upper bounds: These bounds prevent positive-to-positive and negative backward movement of imbalances.

$$v_{ij} \le \begin{cases} x_{N,j} & \text{if } x_{N,j} > 0 \text{ and } x_{N,i} < 0; \\ 0 & \text{otherwise.} \end{cases} \tag{11}$$

Bounds on final imbalances: These bounds ensure that all final imbalances have the "right" sign, i.e. an imbalance must not change sign.

$$\min\{0, x_{N,i}\} \leq y_i \leq \max\{0, x_{N,i}\}, \quad j \in J. \tag{12}$$

Sign on final imbalances: This is a business rule that states that final imbalances for all zones must have the same "sign" (i.e. all nonpositive or nonnegative); that means that the imbalances must not change sign from zone to zone:

$$-M(1-q) \leq y_i \leq Mq, \qquad j \in J, \tag{13}$$

where M is a large number and q is a binary $0-1$ variable.

Shipper's revenue: This equation represents the revenue from the shipper's point of view:

$$z = \sum_{i \in J} r_i y_i + \sum_{(i,j):i<j} b_{ij} v_{ij} - \sum_{(i,j):i<j} f_{ij}(1-e_{ij}) u_{ij}. \tag{14}$$

Variable types:

$$y_i, z \qquad \text{free}; \tag{15}$$

$$u_{ij}, v_{ij} \geq 0; \tag{16}$$

$$q \in \{0, 1\}. \tag{17}$$

In what follows, we will describe the techniques of solution the problem making use of ideas of the penalty method presented in [9].

2.3 Penalty Method

Now we are to apply the penalty function approach to the two resulting *bilevel programs:*

$$\max \qquad h_1(x, s, y, u, v, z) = z, \tag{18}$$

$$\text{subject to (2)–(5) and to} \tag{19}$$

$$\min h_3(x, s, y, u, v, z) = z^2, \tag{20}$$

$$\text{subject to (7)–(16) y} \quad q = 0, \tag{21}$$

and the other which is described by (18)–(21) with $q = 1$ instead of $q = 0$. We consider them as bilevel hierarchical systems in Euclidean space where the upper level decision maker (hereafter the leader) controls a vector of variables $w_1 = (x, s) \in R^{NP} \times R^{NP}$, and the lower level (hereafter the follower) controls a vector of continuous variables $w_2 = (y, u, v) \in R^P \times R^{P(P-1)/2} \times R^{P(P-1)/2}$, and a binary variable $q = \beta$. The leader makes its decision first, taking into account the reaction of the follower to its course of action. If we introduce the function

$$F(y, u, v) = \sum_{i \in J} r_i y_i + \sum_{(i,j):i<j} b_{ij} v_{ij} - \sum_{(i,j):i<j} f_{ij}(1-e_{ij}) u_{ij} \tag{22}$$

and the set

$$W_2^\beta = W_2^\beta(x,s) = \{w_2^\beta = (y,u,v) \text{ defined by (7)-(13),(15)-(16)},\ q=\beta\}, \quad (23)$$

then the reaction $w_2^\beta = w_2^\beta(x,s) = (y,u,v)$ of the follower to the leaders's decision $w_1 = (x,s)$ is a solution to an equilibrium problem represented by the following variational inequality:

$$\langle F(w_2^\beta)\nabla F(w_2^\beta), w_2 - w_2^\beta\rangle \geq 0, \quad \text{for all } w_2 \in W_2^\beta(x,s); \quad (24)$$

here

$$\nabla F(\cdot) = \left((r_i)_{i\in J}, (-f_{ij}(1-e_{ij}))_{(i,j):i<j}, (b_{ij})_{(i,j):i<j}\right)^T. \quad (25)$$

We then obtain the two generalized bilevel programs, or GBLP(β):

$$\text{GBLP}(\beta): \quad F^{\beta,*} = \max_{(x,s)\in W_1,(y,u,v)\in W_2^\beta(x,s)} F(y,u,v),\ \beta = 0,1, \quad (26)$$

subject to (24), where the leader is implicitly restricted to the set W_1 of (x,s)-vectors such that the lower level constraint set $W_2(x,s)^\beta$ be nonempty. Having solved both problems GBLP(0) and GBLP(1), we can then select the final solution of the initial problem between the solutions of the two above-mentioned ones, with respect to the maximality of their optimal values $F^{\beta,*}$, $\beta = 0,1$.

In this paper, we formulate the lower level variational inequality as a parameterized equation related to the duality gap of the lower level problem. We then use this "gap" function as a penalty term for the upper level problem. Since the gap function characterizing the lower level is nonnegative over the feasible domain, the penalty term assumes a very simple form.

Namely, we associate with the lower level variational inequality (24) the *gap function*

$$G_\alpha^\beta(w_1, w_2^\beta) = \max_{w_2\in W_2^\beta(x,s)} \phi(w_1, w_2^\beta, w_2), \quad (27)$$

where

$$\phi(w_1, w_2^\beta, w_2) = -\langle F(w_2^\beta)\nabla F(w_2^\beta), w_2 - w_2^\beta\rangle - \frac{1}{2}\alpha\|w_2 - w_2^\beta\|^2, \quad (28)$$

and α is a positive number. The gap function has been used to construct descent methods for solving variational inequalities. We refer in particular to [7],[8] for the linear gap function ($\alpha = 0$), and to [2] for the quadratic, differentiable function ($\alpha > 0$).

The function ϕ is concave in w_2 (strongly concave if α is positive). Also, since G_α^β is nonnegative over $S_\beta = \bigcup_{w_1\in W_1} w_1 \times W_2^\beta(w_1)$, and $G_\alpha^\beta(w_1, w_2^\beta) = 0$ if and only if w_2^β is a solution to the lower level variational inequality parameterized by (x,s), variational inequality (24) can be rewritten as the nonlinear equation

$$G_\alpha^\beta(w_1, w_2^\beta) = \max_{w_2\in W_2^\beta(x,s)} \phi(w_1, w_2^\beta, w_2) = \phi(w_1, w_2^\beta, p_\alpha(w_1, w_2^\beta)) = 0, \quad (29)$$

where $p_\alpha(w_1, w_2^\beta)$ is any solution of (27). Finally, this leads to a reformulation of the GBLP(β) as the standard mathematical problem

$$\text{PR1}(\beta): \quad \max_{w_1=(x,s)\in W_1, w_2^\beta=(y,u,v)\in W_2^\beta(x,s)} F(y,u,v), \tag{30}$$

$$\text{subject to} \quad G_\alpha^\beta(w_1, w_2^\beta) = 0. \tag{31}$$

3 Inexact Penalization Algorithms

In order to implement the penalty approach, we will approximate PR1(β) by the penalized problem (cf. [9]):

$$\text{PR2}(\beta): \quad \min_{(w_1, w_2^\beta)\in C_\beta} Q_\alpha(w_1, w_2^\beta, \mu), \tag{32}$$

where

$$Q_\alpha(w_1, w_2^\beta, \mu) = -F(w_2^\beta) + \mu G_\alpha^\beta(w_1, w_2^\beta), \tag{33}$$

μ is a positive number, and the subset C_β is such a set in R^{P^2+2NP} that

$$C_\beta = \left\{(w_1, w_2^\beta) \ : \ (2)-(5), (7)-(13), (15)-(16), q=\beta\right\}. \tag{34}$$

Lemma 1. *The subset C_β is convex and compact for each $\beta = 0, 1$.*

Proof. It is easy to see that the constraints (2)–(3) imply that the values of the variables (x, s) are bounded, whereas the values of y belongs to the cube $[-M, M]^P$ (cf. (13)). The values of variables u and v are bounded since they satisfy (10), (11) and (16), and values of $x_{N,j}$ are also bounded. Therefore, the subset C_β is bounded, and being closed it is compact.

To prove the convexity of C_β notice that all the constraints that define C_β are linear, with except constraints (10), (11) and (12). But it is evident that combined with (16), both (10) and (11) obtain the convex subsets. Finally, although (12) define a non-convex subset, they deliver convex subsets combined with (13). Thus, the subset C_β is convex which completes the proof. ■

Therefore, problem PR2(β) is nonlinear with convex constraints, and its objective function is continuously differentiable when α is positive. For each value of the weight μ we denote by $\left(w_1(\mu), w_2^\beta(\mu)\right)$ a global optimal solution of PR2(β) which always exists due to the convexity of the feasible set C_β and continuity of the objective function Q_α. A penalty function algorithm is obtained by specifying a sequence of increasing (unbounded) positive weights $\{\mu_k\}$ and the associated sequence of iterates $\left\{\left(w_1(\mu_k), w_2^\beta(\mu_k)\right)\right\}$.

Below we state a convergence result for the penalty function algorithm, making use of the corresponding techniques from [9]. We omit the proof of the theorem as it almost repeats that of Proposition 1 in [9].

Theorem 1. *Let* $\left\{\left(w_1^k, w_2^k\right)\right\}_{k=1}^{\infty}$ *be a sequence of iterates generated by a penalty function algorithm based upon the function* Q_α *from program PR2*(β).

Then every limit point of the sequence $\left\{\left(w_1^k, w_2^k\right)\right\}_{k=1}^{\infty}$ *is a solution of the bilevel program PR1*(β).

Remark 1. After having obtained two optimal solutions $\left(\bar{w}_1^\beta, \bar{w}_2^\beta\right)$ to the problems PR1(β), $\beta = 0, 1$, we can find the optimal solution of the initial problem (1)–(5), (6)–(17) as follows:

$$(w_1^*, w_2^*) = \begin{cases} \left(w_1^0, w_2^0\right), & \text{if } F\left(w_2^0\right) \geq F\left(w_2^1\right), \\ \left(w_1^1, w_2^1\right), & \text{otherwise.} \end{cases} \tag{35}$$

4 Conclusions and Directions of Future Research

In this paper, we present a mathematical framework for the problem of minimizing the cash-out penalties from the point of view of the natural gas shipper. The problem is modeled as a mixed bilevel linear programming problem. To solve it efficiently, we reformulate it as a standard mathematical programming problem and describe an algorithm of penalty functions for its solution. The algorithm is well-founded and its convergence is proved.

In the next step of our research activity, we are going to demonstrate that actually, the initial problem can be splitted into two almost independent subproblems. Solution set of the first subproblem consists of all feasible imbalances on the last day of the term, each of which, in its turn, can be chosen as an initial iterate for the second subproblem, the bilevel leader-follower one. The first subproblem can be solved by general methods of linear programming but we hope to develop a specialized algorithm to solve it, which would take into account the special structure of the subproblem in question.

The second subproblem must be solved by iterative methods based on penalty functions. In this paper, we have obtained the convergence results for the inexact penalty function algorithm, when there is no finite value of the parameter μ for which the solution of the penalized problem agrees with the optimal solution of GBLP(β). In our future research activity we hope to provide results concerning the exactness preperty of the penalization scheme based on the "classical" gap function introduced by Hearn [3] in an optimization setting and corresponding to the choice $\alpha = 0$ in P1(β), in both cases of separable and non-separable constraints. Results of this kind were obtained in [9] but only for linear constraints. Since not all the constraints in our initial problem are linear, those results of [9] are not applicable directly to our problem.

The next step of is to reduce the bilevel problem GBLP(β) to a bilevel variational inequality making use of the derivative of the initial objective function. To thus obtained bilevel variational inequality one can apply the penalty techniques (cf. [6]).

From a practical point of view, the nonconvex and nondifferentiable (when $\alpha = 0$) problems PR1(β) and PR2(β) are difficult to solve. Recently, in the context of linear bilevel programming, Gendreau et al. [4] proposed an efficient heuristic for generating a high-quality initial solution, later to be used as a starting point for local search methods. This procedure was based on a primal-dual, exact penalty formulation of the linear bilevel program. This techniques can be adapted within a nonlinear framework, too. In the next step of our research activity, we will conduct test and practical computing experiments with the problem of cash-out minimization described above. One of the targets will also be the application of the optimal or quasi-optimal accuracy control realized at the iterations of the algorithm. When one is quite far from the optimal solution one need not fulfil the intermediate steps with too strict accuracy. An optimal strategy of control of the accuracy at the lower level steps was proposed in [5] for general bilevel processes. Now we are going to apply these general techniques to the problems in question.

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