RC24213 (W0703-042) March 9, 2007
Mathematics

IBM Research Report

MINLP Strengthening for Separable Convex Quadratic Transportation-Cost UFL

Oktay Günlük, Jon Lee
IBM Research Division
Thomas J. Watson Research Center
P.O. Box 218
Yorktown Heights, NY 10598

Robert Weismantel
Otto-von-Guericke Universität Magdeburg

MINLP Strengthening for Separable Convex Quadratic Transportation-Cost UFL

Oktay Günlük[1], Jon Lee[1], Robert Weismantel[2]

[1] IBM T.J. Watson Research Center
[2] Otto-von-Guericke Universität Magdeburg

March 8, 2007

Abstract

In the context of a variation of the standard UFL (Uncapacitated Facility Location) problem, but with an objective function that is a separable convex quadratic function of the transportation costs, we present some techniques for improving relaxations of MINLP formulations. We use a disaggregation principal and a strategy of developing model-specific valid inequalities (some nonlinear), which enable us to significantly improve the quality of the NLP (Nonlinear Programming) relaxation of our MINLP model. Additionally, we describe some directions in which our methodology can be extended.

Keyword(s): facility location, mixed integer nonlinear programming, outer approximation

Introduction

The general form of an MINLP (Mixed Integer NonLinear Programming) problem that we consider is

$$\text{P:} \qquad \begin{aligned} &\min\ f(x,y) \\ &\quad \text{subject to:} \\ &\qquad g_i(x,y) \le b_i \ , \ \text{for } i = 1,2,\ldots,p \ , \\ &\qquad x \in \mathbb{R}^{n_{\mathbb{R}}} \ , \ y \in \mathbb{Z}^{n_{\mathbb{Z}}} \ , \end{aligned}$$

where $f : \mathbb{R}^{n_{\mathbb{R}}} \times \mathbb{R}^{n_{\mathbb{Z}}} \mapsto \mathbb{R}$ and the $g_i : \mathbb{R}^{n_{\mathbb{R}}} \times \mathbb{R}^{n_{\mathbb{Z}}} \mapsto \mathbb{R}$ $(i = 1,2,\ldots,p)$ are convex (and typically twice continuously differentiable) functions.

Let $\mathrm{P_R}$ denote the NLP relaxation of P. Convexity of the functions implies that $\mathrm{P_R}$ is a convex program. We are particularly interested in situations where (i) the solution of $\mathrm{P_R}$ does not tend to be on the boundary of its feasible region, and (ii) P has some structure that we can take advantage of. Because of (i), the traditional cutting-plane approaches (both generic cuts like MIR and problem-specific cuts) in the space of the model variables, which are successful for MILP (Mixed Integer Linear Programming), will not be useful here. One approach for such problems is the MINLP approach of OA (Outer Approximation), wherein we minimize a real variable ϕ, subject to the constraints of P as well as the constraint $f(x,y) \le \phi$. As the objective function is now linear, and since we still have a convex relaxation, the optimal solution is now on the boundary of the feasible region of the relaxation. Then generic cutting planes of the OA method may be fruitfully applied (see [4]). Moreover, OA and other methods like NLP-based Branch-and-Bound may benefit from valid inequalities that tighten the relaxation $\mathrm{P_R}$.

In what follows, from the above point of view, we study a variant of the UFL (Uncapacitated Facility Location) problem. In our variant, the objective function is linear on the facility variables as is usual, but we allow for nonlinear convex dependence on the shipment variables.

We attack our problem by proceeding in the spirit of OA, but we refine the approach by (i) disaggregating the objective function by introducing new variables corresponding to different nonlinear parts of the objective function that are added together, and then (ii) establishing problem-specific valid inequalities — some valid for the set of feasible solutions, and some only valid on the set of optimal solutions. We note that some of our inequalities are nonlinear (but convexity preserving). We are of course motivated by the success of disaggregation and developing model-specific cutting planes — two very useful principals from MILP (see [13], for example). Our approach appears to be quite general, but we mainly focus on a variant of the UFL problem for the sake of concreteness.

We note that there has been considerable work on other nonlinear versions of facility location problems (see [6, 10, 11, 12, 15, 16, 14] for example), but the models and methods are quite different from what we investigate.

In Section 1, we introduce our variant of the UFL. In Section 2, we develop our techniques in the context of the separable quadratic-cost UFL. Section 3 contains the results of successful computational experiments. Finally, in Section 4 we describe an extension.

1 The UFL problem

Given a set of "customers" $N := \{1, 2, \ldots, n\}$ with demand for a single commodity and a set of potential "facilities" $M := \{1, 2, \ldots, m\}$ with unlimited capacity, the *Uncapacitated Facility Location* (UFL) problem involves (i) choosing a subset of the facilities to open and (ii) determining how much of each customer's demand is satisfied by each open facility. The objective function consists of transportation costs as well as fixed costs associated with opening facilities.

To model the problem, we define a 0/1-valued variable

$$y_i := \text{indicator variable for whether or not facility } i \text{ is open,}$$

for each $i \in M$, and a continuous variable

$$x_{ij} := \text{fraction of demand of customer } j \text{ satisfied by facility } i \ .$$

for each $i \in M$ and $j \in N$. For notational convenience, we also define $x_{\cdot j} \in \mathbb{R}^m$ to denote the column vector $(x_{1j}, x_{2j}, \ldots, x_{mj})^T$.

We next define the UFL problem with partially-separable transportation costs:

$$\mathrm{P}_{\mathrm{UFL}}: \quad \begin{array}{lll} \min & c^T y + \sum_{j \in N} f_j(x_{\cdot j}) & \\ \text{subject to:} & & \\ & \mathbf{0} \le x_{\cdot j} \le y \ , & \text{for } j \in N \ , \\ & \mathbf{e}^T x_{\cdot j} = 1 \ , & \text{for } j \in N \ , \\ & y_i \in \{0, 1\} \ , & \text{for } i \in M \ , \end{array}$$

where c_i is the cost of opening facility $i \in M$, and $f_j : \mathbb{R}^M \mapsto \mathbb{R}$ gives the total transportation cost for customer $j \in N$. As is standard, for a nonempty subset S of M or N, we define $\mathbb{R}^S$ to be $\mathbb{R}^{|S|}$, but with coordinates indexed from S .

Note that if y is fixed to say $\bar{y} \in \{0, 1\}^M$, where $\bar{y} \neq \mathbf{0}$, then the problem decomposes by customer, and it suffices to solve the distribution problem

$$\mathrm{P}^j_{\mathrm{Dist}} \quad \begin{array}{ll} \min & f_j(x_{\cdot j}) \\ \text{subject to:} & \\ & \mathbf{0} \le x_{\cdot j} \le \bar{y} \ , \\ & \mathbf{e}^T x_{\cdot j} = 1 \ , \end{array}$$

for each customer $j \in N$.

For certain objective functions, the distribution problem defined by $\mathrm{P}^j_{\mathrm{Dist}}$ can be solved easily. We next discuss some of these cases. For $\bar{y} \in \{0, 1\}^M$, let $S(\bar{y}) := \{i \in M \ : \ \bar{y}_i = 1\}$.

1.1 Linear Case

The simplest situation is the linear case

$$f_j(x_{\cdot j}) := q_{\cdot j}^T x_{\cdot j} \ ,$$

where q_{ij} denotes the cost of satisfying customer j demand (fully) from facility i . In this case, it is clear (and well known) that optimal solution of $\mathrm{P}^j_{\mathrm{Dist}}$ can be obtained by choosing an open facility $k \in S(\bar{y})$, such that

$$q_{kj} = \min\{q_{ij} \ : \ i \in S(\bar{y})\} \ ,$$

letting $x_{kj} = 1$, and letting $x_{ij} = 0$ for $i \neq k$.

1.2 Quadratic Case

Another nice case is when

$$f_j(x_{\cdot j}) := x_{\cdot j}^T Q_j x_{\cdot j} \ , \tag{1}$$

where Q_j is a symmetric positive definite matrix and therefore f_j is strictly convex.

For nonempty $S \subseteq M$, let $Q_j[S]$ be the principal submatrix of Q_j indexed by S . In addition, let x_{Sj} denote the (column) vector consisting of the $|S|$ components x_{ij} with $i \in S$. It is not to difficult to establish the following lemma using the KKT conditions.

Lemma 1.1. *Suppose f_j has the form (1) and let $\bar{x}_{\cdot j}$ be an optimal solution to $\mathrm{P}^j_{\mathrm{Dist}}$. If $(Q_j[S(\bar{y})])^{-1}$ is diagonally dominant, that is, if $(Q_j[S(\bar{y})])^{-1}\mathbf{e} > 0$, then $\bar{x}_{\cdot j}$ is given by $\bar{x}_{ij} = 0$ for $i \in M \setminus S(\bar{y})$ and*

$$\bar{x}_{ij} = \frac{e_i^T \left(Q_j[S(\bar{y})]\right)^{-1} \mathbf{e}}{\mathbf{e}^T \left(Q_j[S(\bar{y})]\right)^{-1} \mathbf{e}} \ ,$$

for $i \in S(\bar{y})$.

Proof. First note that the objective function f_j is convex on $\mathbb{R}^M_+$, in addition, $\bar{x}_{\cdot j}$ is feasible for $\mathrm{P}^j_{\mathrm{Dist}}$. Furthermore $\bar{x}_{\cdot j}$ satisfies $\nabla f_j(\bar{x}_{\cdot j}) = \lambda \mathbf{e}$ for

$$\lambda = \frac{2}{\mathbf{e}^T \left(Q_j[S(\bar{y})]\right)^{-1} \mathbf{e}} \ ,$$

and therefore $\bar{x}_{\cdot j}$ and λ give a solution to the KKT conditions. □

Note that the hypothesis could be strengthened to simply require that $Q_j^{-1}\mathbf{e}$ be all positive. Also note that under the assumptions of Lemma 1.1 it is easy to see that the optimal value of $\mathrm{P}^j_{\mathrm{Dist}}$ is

$$f_j(\bar{x}_{[j]}) = \frac{1}{\mathbf{e}^T (Q_j[S(\bar{y}]))^{-1} \mathbf{e}} \ .$$

1.3 Simple Polynomial Case

The last case we consider is the simple polynomial case where the objective function has the form

$$f_j(x_{\cdot j}) := \sum_{i \in M} q_{ij} x_{ij}^r \ , \tag{2}$$

for some $r > 0$. All q_{ij} are assumed to be strictly positive. Notice that when $r \leq 1$, f_j is concave on $\mathbb{R}_+$ and in this case (as in the linear case) the optimal solution of $\mathrm{P}^j_{\mathrm{Dist}}$ can be obtained by simply choosing an open facility $k \in S(\bar{y})$, such that

$$q_{kj} = \min\{q_{ij} \ : \ i \in S(\bar{y})\} \ ,$$

letting $x_{kj} = 1$, and letting $x_{ij} = 0$ for $i \neq k$. Next, we analyze the case when $r > 1$.

Lemma 1.2. *Suppose f_j has the form (2), and let $\bar{x}_{\cdot j}$ be an optimal solution to $\mathrm{P}^j_{\mathrm{Dist}}$. If $r > 1$, then $\bar{x}_{\cdot j}$ is given by $\bar{x}_{ij} = 0$ for all $i \in M \setminus S(\bar{y})$, and*

$$\bar{x}_{ij} = \frac{{q_{ij}}^{-1/r-1}}{\sum_{k \in S(\bar{y})} {q_{kj}}^{-1/r-1}} \ ,$$

for $i \in S(\bar{y})$.

Proof. First note that when $r > 1$, the objective function f_j is convex on $\mathbb{R}_+$. In addition, $\bar{x}_{\cdot j}$ is feasible for $\mathrm{P}^j_{\mathrm{Dist}}$, and it satisfies

$$r \, q_{ij} \, \bar{x}_{ij}^{r-1} = \frac{r}{\sum_{k \in S(\bar{y})} {q_{kj}}^{-1/r-1}} \ ,$$

where the right-hand side of the equation does not depend on i and it can be interpreted as the dual multiplier associated with the gradient of the constraint $\sum_{i \in M} x_{ij} = 1$. We therefore have $\nabla f_j(\bar{x}_{\cdot j}) = \lambda e$ for some $\lambda \in \mathbb{R}$ and $\bar{x}_{\cdot j}$ and λ indeed satisfy the KKT conditions. □

Note that under the assumptions of Lemma 1.2, the value of the optimal solution becomes

$$f_j(\bar{x}_{\cdot j}) \ = \ \sum_{i \in S(\bar{y})} q_{ij} (\bar{x}_{ij})^r = \frac{\sum_{i \in S(\bar{y})} q_{ij} \cdot {q_{ij}}^{-r/r-1}}{\left(\sum_{i \in S(\bar{y})} {q_{ij}}^{-1/r-1}\right)^r} = \left(\sum_{i \in S(\bar{y})} {q_{ij}}^{-1/r-1}\right)^{-(r-1)} \ .$$

2 Separable Quadratic UFL

In this section, we study the UFL when the objective function has the form (1) and (2) simultaneously. In other words we now consider the *separable quadratic* case when

$$f_j(x_{\cdot j}) := \sum_{i \in M} q_{ij} x_{ij}^2 \ , \tag{3}$$

where $q_{ij} > 0$ for all $i \in M$ and $j \in N$.

In this case the problem can be reformulated as

$$
\mathrm{P}^{\mathrm{SQ}}_{\mathrm{UFL}} \qquad
\begin{array}{ll}
\min & c^T y + \sum_{j \in N} \phi_j \\
\text{subject to:} & \\
& \sum_{i \in M} q_{ij} x_{ij}^2 \le \phi_j \ , \text{ for } j \in N \ , \\
& \mathbf{0} \le x_{\cdot j} \le y \ , \qquad \text{for } j \in N \ , \\
& \mathbf{e}^T x_{\cdot j} = 1 \ , \qquad \text{for } j \in N \ , \\
& y \in \{0,1\}^M \ .
\end{array}
$$

where we introduce real variables ϕ_j, one for each customer $j \in N$, to move the nonlinearity from the objective into the constraints.

For the UFL problem with linear objective function, it is well known (see [13], for example) that the continuous relaxation of the problem gives a very good approximation of the mixed-integer problem, and therefore simple branch-and-bound techniques can be employed to solve the problem to optimality. In the separable quadratic case, however, this is not the case as the continuous relaxation of the problem is quite weak. In the remainder of this section we present valid inequalities (that involve the ϕ variables) to tighten the continuous relaxation of $\mathrm{P}^{\mathrm{SQ}}_{\mathrm{UFL}}$.

It is also worth noting that unlike the linear case, using the *aggregated formulation* (where the constraints $x_{ij} \le y_i$ for $j \in M$ are aggregated into a single constraint $\sum_{j \in M} x_{ij} \le m\, y_i$) does not effect the quality of the continuous relaxation significantly. In fact, there is theoretical (see [9]) and computational (see [8]) evidence that the aggregated formulation may actually be preferred for convex nonlinear objective functions.

As the separable quadratic case lies in the intersection of the quadratic case (by setting $Q_j = \mathrm{diag}(q_{1j}, q_{2j} \ldots, q_{mj})$) and the simple polynomial case (by setting $r = 2$) the distribution problem $\mathrm{P}^{j}_{\mathrm{Dist}}$ can be solved easily.

Corollary 2.1. *Let (x', y', ϕ') be an optimal solution to $\mathrm{P}^{\mathrm{SQ}}_{\mathrm{UFL}}$. Then,*

$$
x'_{ij} = \frac{1/q_{ij}}{\sum_{l \in S(y')} 1/q_{lj}} y'_i \quad \text{and} \quad \phi'_j = \frac{1}{\sum_{l \in S(y')} 1/q_{lj}} \ .
$$

By Corollary 2.1, optimal solutions to $\mathrm{P}^{\mathrm{SQ}}_{\mathrm{UFL}}$ satisfy the nonlinear equations

$$
\phi_j y_i = q_{ij} x_{ij} \ , \tag{4}
$$

for all $i \in M$ and $j \in N$.

Based on this observation, it is possible to derive a *linear* formulation of the problem. It is easy to see that the linear formulation presented in Lemma 2.2 is a relaxation of the problem as the optimal solution (x', y', ϕ') of $\mathrm{P}^{\mathrm{SQ}}_{\mathrm{UFL}}$ is also feasible for $\bar{\mathrm{P}}^{\mathrm{QS}}_{\mathrm{UFL}}$ and has the same objective value.

Lemma 2.2. *The following gives an MILP reformulation of* $\mathrm{P}^{\mathrm{SQ}}_{\mathrm{UFL}}$*:*

$$\bar{\mathrm{P}}^{\mathrm{QS}}_{\mathrm{UFL}} \qquad \begin{aligned} \min \quad & c^T y + \sum_{j \in N} \phi_j \\ \text{subject to:} & \\ & q_{ij} x_{ij} \le \phi_j \ , \ \textit{for } i \in M, \ j \in N, \\ & \mathbf{0} \le x_{\cdot j} \le y \ , \ \textit{for } j \in N, \\ & \mathbf{e}^T x_{\cdot j} = 1 \ , \quad \textit{for } j \in N, \\ & y \in \{0,1\}^M \ . \end{aligned}$$

Proof. Let (x', y', ϕ') be an optimal solution to $\bar{\mathrm{P}}^{\mathrm{QS}}_{\mathrm{UFL}}$ and consider a fixed $j \in N$. We will demonstrate that ϕ'_j measures the flow cost correctly and therefore establish that optimal value of $\mathrm{P}^{\mathrm{SQ}}_{\mathrm{UFL}}$ and $\bar{\mathrm{P}}^{\mathrm{QS}}_{\mathrm{UFL}}$ are the same.

Clearly $x'_{ij} = 0$ for all $i \notin S(y')$ and $q_{kj} x'_{kj} = \phi_j$ for some $k \in S(y')$. In addition, unless $q_{ij} x'_{ij} = \phi_j$ for all $i \in S(y')$, objective value can be improved and therefore (x', y', ϕ') could not be an optimal solution. To see this notice that if $q_{ij} x'_{ij} < \phi'_j$ for some $i \in S(y')$, increasing x'_{ij} and decreasing all x'_{kj} for $k \in S(y') \setminus \{i\}$ would decrease ϕ'_j .

As $x'_{ij} = \phi'_j / q_{ij}$ for all $i \in S(y')$, we have

$$\sum_{i \in M} x'_{ij} = \phi'_j \sum_{i \in S(y')} 1/q_{ij} = 1 \ ,$$

and therefore ϕ' indeed has the correct value shown in Corollary 2.1. □

It is important to note that this linear formulation is based on optimality conditions and as such would not generally be a valid formulation when there are additional constraints on the x and y variables. In addition, this formulation has a min-max structure which makes it rather hard for MILP solvers.

2.1 VUB inequalities

We can linearize and then strengthen (4) to obtain

$$q_{ij} x_{ij} + (1 - y_i) / \sum_{l \in M - i} 1/q_{lj} \le \phi_j \ , \tag{5}$$

which we call the *strengthened variable upper bound inequality.*

Lemma 2.3. *For all* $i \in M$ *and* $j \in N$*, the strengthened variable upper bound inequality 5 is valid for all feasible solutions of* $\mathrm{P}^{\mathrm{SQ}}_{\mathrm{UFL}}$*.*

Proof. If $y_i = 1$, the inequality reduces to $q_{ij} x_{ij} \le \phi_j$ which is implied by (4). On the other hand, if $y_i = 1$, the inequality becomes $\sum_{l \in M - i} 1/q_{lj} \le \phi_j$ which is valid as ϕ_j attains its least value when all facilities are open. □

Note that these inequalities are valid for all feasible solutions even though we use optimality conditions to demonstrate validity.

2.2 Subset customer-cost lower bounds

In this section we develop valid inequalities of the form

$$1/\sum_{j\in S} 1/\phi_j \geq \alpha(x,y) \ ,$$

where S is a nonempty subset of N and α is convex in (x,y) . Actually, α will be a function of y, and linear at that. To demonstrate that inequalities of this form maintain a convex relaxation, we start with the following observation.

Lemma 2.4. *For nonempty $S \subseteq N$, the function $h : \mathbb{R}^{|S|}_{++} \mapsto \mathbb{R}$ defined by $h(v) = 1/\sum_{j\in S} 1/v_j$ is concave.*

Proof. $1/v_j$ is convex on $\mathbb{R}_{++}$. Therefore, the sum $\sum_{j\in S} 1/v_j$ is convex on $\mathbb{R}^{|S|}_{++}$. Therefore, $1/\sum_{j\in S} 1/v_j$ is concave on $\mathbb{R}^{|S|}_{++}$. □

Though $h(v)$ is nonlinear when $|S| > 1$, it is rather well behaved; for example, when $|S| = 2$, $h(v)$ has the graph of Figure 1, which we note is rather flat away from the coordinate axes.

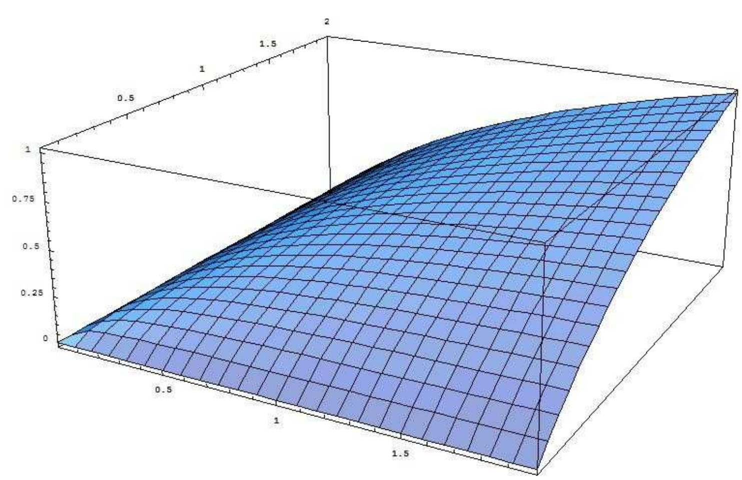

Figure 1: Plot of $\frac{1}{1/v_1+1/v_2}$

Next, we set some convenient notation. For nonempty $S \subseteq N$ and integer k satisfying $1 \leq k \leq m$, let

$$H^k_S := 1/\sum_{i=1}^{k} p_{iS} \ ,$$

where, for $i \in M$, we let

$$p_{iS} := \sum_{j \in S} 1/q_{ij} \ .$$

To simplify notation, we assume that p_{iS} are sorted (for a given S) so that

$$p_{1S} \geq p_{2S} \geq \cdots \geq p_{mS} \ .$$

We next introduce the *simple subset customer-cost lower bound* inequalities.

Lemma 2.5. *Let S be nonempty subset of N and let k be an integer satisfying $1 \leq k \leq m$. The simple subset customer-cost lower bound inequality*

$$1/\sum_{j \in S} 1/\phi_j \geq H_S^k \tag{6}$$

is valid for all feasible solutions of $\mathrm{P}_{\mathrm{UFL}}^{\mathrm{SQ}}$ that satisfy $\sum_{i \in M} y_i = k$. In addition, inequality (6) is convex.

Proof. Convexity of inequality (6) follows from Lemma 2.4. To see validity, notice that when $\sum_{i \in M} y_i = k$,

$$1/\sum_{j \in S} 1/\phi_j \quad \geq \quad \frac{1}{\max\limits_{\substack{Y \subseteq M \\ |Y|=k}} \left\{ \sum_{i \in Y} \sum_{j \in S} 1/q_{ij} \right\}} \quad = \quad \frac{1}{\sum_{i=1}^{k} p_{iS}} \quad = \quad H_S^k \ .$$

□

We note that considering the objective function of $\mathrm{P}_{\mathrm{UFL}}^{\mathrm{SQ}}$, it is more natural to seek to lower bound $\sum_{j \in S} \phi_j$, thus keeping the inequality linear. However, then we do not see how to calculate the appropriate lower bound. So, we use this nonlinear surrogate $1/\sum_{j \in S} 1/\phi_j$, which we know how to lower bound, for $\sum_{j \in S} \phi_j$.

Toward using these simple subset customer-cost lower bounds to form an inequality that does not require $\sum_{i \in M} y_i = k$, we prove that the H_S^k are discrete convex in k .

Lemma 2.6. *Let S be nonempty subset of N and let k be an integer satisfying $1 \leq k \leq m-2$. Then,*

$$H_S^k + H_S^{k+2} \geq 2H_S^{k+1} \ .$$

Proof.

$$
\begin{aligned}
H_S^k + H_S^{k+2} - 2H_S^{k+1} &= \frac{1}{\sum_{i=1}^{k} p_{iS}} + \frac{1}{\sum_{i=1}^{k+2} p_{iS}} - \frac{2}{\sum_{i=1}^{k+1} p_{iS}} \\
&= \left(\frac{1}{\sum_{i=1}^{k+1} p_{iS}}\right)\left(\frac{\sum_{i=1}^{k+1} p_{iS}}{\sum_{i=1}^{k} p_{iS}} + \frac{\sum_{i=1}^{k+1} p_{iS}}{\sum_{i=1}^{k+2} p_{iS}} - 2\right) \\
&= \left(\frac{1}{\sum_{i=1}^{k+1} p_{iS}}\right)\left(1 + \frac{p_{k+1S}}{\sum_{i=1}^{k} p_{iS}} + \frac{\sum_{i=1}^{k+1} p_{iS}}{\sum_{i=1}^{k+2} p_{iS}} - 2\right) \\
&\geq \left(\frac{1}{\sum_{i=1}^{k+1} p_{iS}}\right)\left(1 + \frac{p_{k+2S}}{\sum_{i=1}^{k+2} p_{iS}} + \frac{\sum_{i=1}^{k+1} p_{iS}}{\sum_{i=1}^{k+2} p_{iS}} - 2\right) \\
&= 0\ .
\end{aligned}
$$

□

Finally, we introduce the *subset customer-cost lower bound* inequalities

(7) $$1/\sum_{j\in S} 1/\phi_j \ \geq\ H_S^k\left(k+1-\sum_{l\in M} y_l\right) + H_S^{k+1}\left(-k+\sum_{l\in M} y_l\right).$$

Combining the lemmata, we have the following result.

Theorem 2.7. *Let S be nonempty subset of N and let k be an integer satisfying $1 \leq k \leq m-1$. Then, the subset customer-cost lower bound inequality (7) is valid for all feasible solutions of $\mathrm{P}_{\mathrm{UFL}}^{\mathrm{SQ}}$. In addition, inequality (7) is convex.*

Proof. Convexity of inequality (7) again follows from Lemma 2.4. To see validity, notice that for any integer $\bar{k}$ satisfying $1 \leq \bar{k} \leq m-1$, if $\sum_{l\in M} y = \bar{k}$, then we have

(8) $$1/\sum_{j\in S} 1/\phi_j \ \geq\ H_S^{\bar{k}} \ \geq\ H_S^k\left(k+1-\bar{k}\right) + H_S^{k+1}\left(-k+\bar{k}\right)$$

where the last inequality follows from the fact that H_S^k is convex in k by Lemma 2.6. □

We note that the subset customer-cost lower bounds can be strengthened by increasing the coefficients of some of the y_l . In particular, this can be done for the y_l corresponding to the facility l that is "closest" (according to the p_{lS}) to customer subset S . The form of the expression is a bit complicated, so we do not present it here.

Before continuing, we take a brief detour to place our inequality in a classical mathematical context. Our subset customer-cost lower bound has the form $h(\phi_S) := 1/\sum_{j\in S} 1/\phi_j >= \alpha(y)$. The well-known *harmonic mean* of the ϕ_j , $j \in S$, is just $H(\phi_S) := |S|h(\phi_S)$. Other classical means are the *geometric mean* $G(\phi_S) := \sqrt[|S|]{\prod_{j\in S}\phi_j}$ and of course the *arithmetic mean* $\sum_{j\in S}\phi_j/|S|$.

The classical inequality relating the arithmetic, geometric and harmonic means is simply $A(\phi_S) \geq G(\phi_S) \geq H(\phi_S)$. (with equality if and only if all ϕ_j are equal). So we have

$$A(\phi_S)/|S| \geq G(\phi_S)/|S| \geq H(\phi_S)/|S| \geq \alpha(y) \ .$$

So while the linear inequality $A(\phi_S)/|S| \geq \alpha(y)$ is valid, we can regard our subset customer-cost lower bounds as a nonlinear strengthening of this linear inequality. In between we have the weaker strengthening $G(\phi_S)/|S| \geq \alpha(y)$, which is also a convex inequality, since the geometric mean is concave also.

Finally, we note that our subset customer-cost lower bounds can be viewed as coming from a more general framework that we propose in Section 4.

2.3 Arc-flow lower bounds

Using ideas similar to those in the previous section, we next derive lower bounds on individual x_{ij} variables. The inequality we describe below is not valid for all feasible solutions of $\mathrm{P}^{\mathrm{SQ}}_{\mathrm{UFL}}$. It is however valid for the set of *optimal* solutions.

Let $j \in N$ be given. To simplify notation, we assume that q_{ij} are non-decreasing:

$$q_{1j} \leq q_{2j} \leq \cdots \leq q_{mj} \ .$$

Next, we define

$$L^k_{ij} := \begin{cases} \dfrac{1/q_{ij}}{1/q_{ij} + \sigma^{k-1}_j} \ , & \text{for } i > k \ ; \\ \dfrac{1/q_{ij}}{\sigma^k_j} \ , & \text{for } i \leq k \ , \end{cases}$$

where $\sigma^k_j := \sum_{i=1}^k 1/q_{ij}$.

In correspondence with Lemmata 2.1 and 2.2, we first show that the inequality below is valid when $\sum_{l \in M} y_l = k$. We then show that L^k_{ij} is discrete convex in k .

Lemma 2.8. *Given $i \in M$ and $j \in N$, the simple arc-flow lower bound inequality*

$$x_{ij} \geq L^k_{ij} y_i \tag{9}$$

is valid for optimal solutions satisfying $\sum_{l \in M} y_l = k$.

Proof. Let (x', y', ϕ') be an optimal solution to $\mathrm{P}^{\mathrm{SQ}}_{\mathrm{UFL}}$ that satisfies $\sum_{l \in M} y'_l = k$. If $y'_i = 0$, inequality (9) reduces to the nonnegativity constraint and therefore, is valid. If, on the other hand, $y_i = 1$ then by Lemma 2.1

$$x'_{ij} = \frac{1/q_{ij}}{\sum_{l \in M} (1/q_{lj}) y'_l} \geq L^k_{ij} \ ,$$

where the last inequality follows form the fact that the denominator of the previous expression is maximized when $y'_l = 1$ for $l \in M$ with large $1/q_{lj}$, or, equivalently, with small q_{lj} . □

The simple arc-flow lower bound inequality (9) can also be viewed as a strengthening of the the nonnegativity constraints

$$x_{ij} \geq 0 \cdot y_i \ .$$

when $\sum_{l \in M} y_l = k$.

Lemma 2.9. *Let $i \in M$, $j \in N$ and let k be an integer satisfying $1 \leq k \leq m-2$. Then,*

$$L_{ij}^{k} + L_{ij}^{k+2} \geq 2L_{ij}^{k+1} \ .$$

Proof. Similar to the proof of Lemma 2.6. □

We use these lemmata to establish that the following *arc-flow lower bounds* are valid for all optimal solutions.

Theorem 2.10. *Let $i \in M$, $j \in N$ and $k \in \{1, \ldots, n-1\}$ be given. The arc-flow lower bound inequality*

$$x_{ij} \geq L_{ij}^{k} \left((k+1)y_i - \sum_{l \in M} y_l \right) + L_{ij}^{k+1} \left(-ky_i + \sum_{l \in M} y_l \right) + \left(L_{ij}^{k} - L_{ij}^{k+1} \right) (1 - y_i) \ ,$$

is valid for all optimal solutions.

Proof. We consider two cases. When $y_i = 1$, the inequality reduces to

$$x_{ij} \geq L_{ij}^{k} \left(1 + k - \sum_{l \in M} y_l \right) + L_{ij}^{k+1} \left(-k + \sum_{l \in M} y_l \right),$$

the validity of which follows from Lemmata 2.8-2.9.

Alternatively, when $y_i = 0$, the inequality reduces to

$$x_{ij} \geq \left(L_{ij}^{k} - L_{ij}^{k+1} \right) \left(1 - \sum_{l \in M : l \neq i} y_l \right),$$

in which the right-hand side is non-positive since the L_{ij}^{k} are decreasing in k, and at least one facility must be open to satisfy demand. □

We note that similar results can be obtained for *upper* bounds on x_{ij}, but we expect such inequalities to be less useful in practice.

One possible computational strategy for solving our problem is to enumerate on $k = \sum_{l \in M} y_l$. If we do add this equation, then the arc-flow (resp., customer-cost) lower bounds reduce to the simple arc-flow (resp., customer-cost) lower bounds.

3 Computational experiments

We performed some computational experiments using the open-source MINLP code Bonmin 0.1, which is distributed on COIN-OR (see [1] for a description of the algorithm; the users' manual [2] and source code are available at [3]). For our computational results, we used the B&B (branch-and-bound) algorithmic option of Bonmin and otherwise accepted the defaults (e.g., the default node selection strategy is 'best bound'), including use of the NLP interior-point solver Ipopt [7]. We note that preliminary experiments indicated that B&B is a better choice for our instances than OA. We used AMPL [5] to interface with Bonmin. Our experiments were carried out on a dual-processor machine with 2 GHz AMD Opterons and equipped with 3GB of memory.

Figure 2 illustrates an experiment that we made for a difficult separable quadratic UFL. This instance from [8], has 30 potential facilities and 100 customers. We solved 30 subproblems, each of which fixes the number of facilities to open to a specific number k (i.e., we appended the constraint $\sum_{i \in M} y_i = k$) for all possible choices of $k = 1, 2, \ldots, 30 (= m)$. The bottom of the three curves indicates the optimal objective value of the NLP relaxation. The top curve indicates the optimal value of the MINLP. It is noteworthy that the optimal solution of the NLP relaxation suggests that opening one facility is optimal, giving us no real hint at the optimal number of facilities, which happens to be eight. The middle curve reflects the improvement in the relaxation using our inequalities. In particular, we utilized: strengthened VUBs, arc-flow lower bounds, subset customer-cost lower bounds for all subsets S with $|S| \in \{1, n-1, n\}$ and some S with $|S| = 2$.

We were interested in seeing the value of our inequalities to improve B&B. Table 1 indicates the improvement in the NLP lower bound achieved by our inequalities, across five problems of varying size. In regard to Table 1, we successively compare the value of different types of inequalities. Details of what we compare are summarized as follows:

- Base Model: $\mathrm{P}^{\mathrm{SQ}}_{\mathrm{UFL}}$;
- w/ Linear Cust-Cost: Additionally, with subset customer-cost lower bounds for all singleton sets S ;
- w/ Nonlin Cust-Cost: Additionally, with subset customer-cost lower bounds for all S with $|S| = n-1, n$ and some S with $|S| = 2$. In particular, we used these for $|S| = 2$ only when the distance between the pair of facilities constituting S was greater than some cutoff.
- w/ VUB & Arc-Flow: Additionally, with strengthened VUBs and arc-flow lower bounds;
- Opt: The optimal objective value (obtained by Bonmin's B&B).

Table 1 demonstrates that our inequalities cut down between 70 and 90 percent of the gap between the optimum and the lower bound obtained by using the original NLP relaxation. We note that we only employed a limited subset of the subset customer-cost lower bounds, so there is significant potential to improve the bounds further.

Table 2 indicates the performance of Bonmin's B&B in solving problems to optimality. Apparently, our inequalities are useful in limiting the B&B search. But it should be noted that inclusion of all of our inequalities slows down the NLP solver rather drastically. We note that the nearly 10-fold decrease in the node count for the $m = 30, n = 100$ problem, was obtained using only the subset

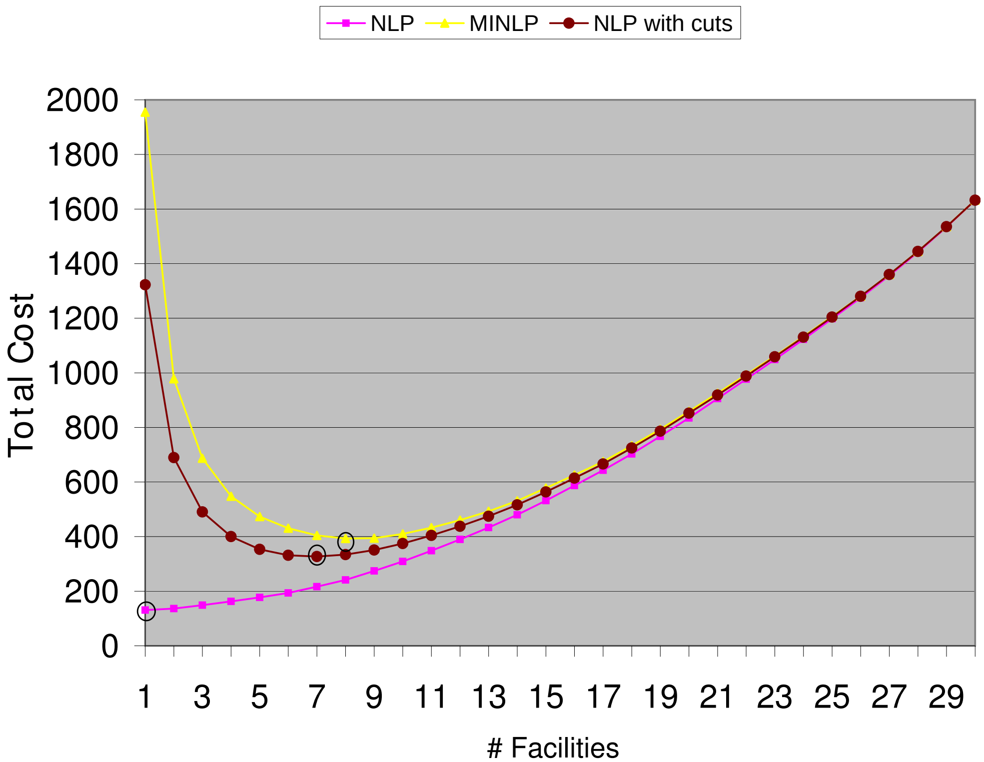

Figure 2: Bound performance

customer-cost lower bounds for $|S| = n$ on top of the base formulation. For this instance, our inequalities reduced the running time by about 80% . Still, we need to find a way to solve the NLP subproblems faster, so that we can fully realize the power of our inequalities; there are many possibilities here (e.g., using looser tolerances in Ipopt, using an active-set based NLP solver rather than Ipopt, using an OA algorithm rather than B&B, using cuts very selectively, aggregating cuts, etc.), and this is work in progress.

4 UFL with more general convex costs

So as to suggest the potential generality of some of our techniques, we consider a more general form of the $f_j(x_{\cdot j})$, with the goal of generalizing the subset customer-cost lower bounds for the case in which the subset S consists of a singleton j . We assume that

$$f_j(x_{\cdot j}) := \sum_{i \in M} q_{ij} \zeta_j(x_{ij}) ,$$

where the q_{ij} are positive, and $\zeta_j : [0,1] \mapsto \mathbb{R}$ is continuously differentiable and convex. So f_j attains its minimum at a KKT point. Let $q_{\min(j)} := \min\{q_{ij} \ : \ i \in M\}$ and $q_{\max(j)} := \max\{q_{ij} \ : \ i \in M\}$.

m, n	Base Model	w/ Linear Cust-Cost	w/ Nonlin Cust-Cost	w/ VUB & Arc-Flow	Opt
10,30	140.555	286.809	324.227	326.444	348.777
15,50	141.282	261.407	305.915	312.200	384.087
20,65	122.512	206.930	242.948	248.689	289.324
25,80	121.315	201.437	256.031	260.073	315.803
30,100	128.048	248.080	322.658	327.005	393.154

Table 1: Effectiveness of our inequalities: objective values

m,n	No cuts	Some cuts
10,30	384	118
15,50	1386	498
20,65	982	178
25,80	4,638	928
30,100	29,272	3,250

Table 2: Effectiveness of our inequalities: Node counts

We further assume that

$$0 \le \zeta_j'(0) < \frac{q_{\min(j)}}{q_{\max(j)}} \zeta_j'(\tfrac{1}{m-1}) \ . \tag{10}$$

It is easy to check that for example $\zeta_j(x_{ij}) = a_j + \sum_t x_{ij}^{r_{jt}}$, with $a_j \in \mathbb{R}$, $r_{jt} \in \mathbb{R}$, $r_{jt} > 1$ satisfies this condition.

Let

$$P_j : \quad \begin{aligned} & z_j^k := \min \sum_{i \in M} q_{ij} \zeta_j(x_{ij}) \\ & \text{subject to:} \\ & \mathbf{e}^T x_{\cdot j} = 1 \ ; \\ & 0 \le x_{\cdot j} \le y \ ; \\ & \mathbf{e}^T y = k \ ; \\ & y_i \in \{0,1\} \ , \ \forall \ i \in M \ ; \end{aligned}$$

Assume that the q_{ij} are sorted so that

$$q_{1j} \le q_{2j} \le \cdots \le q_{mj} \ .$$

Lemma 4.1. *If (10) holds, then there is an optimal solution to P_j having $y_i = 1$ and $x_{ij} > 0$ for $1 \le i \le k$, and $y_i = x_{ij} = 0$ for $k+1 \le i \le m$.*

Proof. By the symmetry over i in the constraints and that we have sorted the q_{ij} , it is clear that there is an optimal solution with $y_i = 1$ for $1 \le i \le k$, and $y_i = x_{ij} = 0$ for $k+1 \le i \le m$. Moreover, again by how the q_{ij} are sorted, we can assume that $x_{1j} \ge x_{2j} \ge \cdots \ge x_{kj}$. Let k' be the least i for which $x_{k'j} = 0$. We assume that $k' (\le k)$ exists, or we are done. Clearly $x_{1j} \ge \frac{1}{k'-1}$.

We will demonstrate how to construct a solution having an additional component positive and with lower objective value. Consider the solution obtained from $x_{\cdot j}$ by letting $x_{k'j} = \epsilon$ and decreasing x_{1j} by ϵ, for some small positive ϵ . The change in the objective value is

$$-q_{1j}\zeta_j'(x_{1j})\epsilon + q_{k'j}\zeta_j'(0)\epsilon + O(\epsilon^2) \ .$$

This is negative, for sufficiently small $\epsilon > 0$ since

$$\frac{\zeta_j'(0)}{q_{1j}} < \frac{\zeta_j'(\frac{1}{m-1})}{q_{mj}} \leq \frac{\zeta_j'(\frac{1}{k'-1})}{q_{k'j}} \leq \frac{\zeta_j'(x_{1j})}{q_{k'j}} \ ,$$

this first inequality holding by (10), the second holding since ζ_j' is nondecreasing and the q_{ij} are non-decreasing in i, and the last holding since ζ_j' is non-decreasing. □

Therefore, our hypothesis (10) implies that we can solve the MINLP P_j by solving an NLP. Since we know that $x_{\cdot j}$ is all positive, our hypothesis (10) implies that the KKT system for the NLP reduces to:

$$q_{ij}\zeta_j'(x_{ij}) = v_j^k \ , \quad \forall \ i \ .$$

It is an easy matter to solve this nonlinear system of equations via a bisection search on v_j^k .

We compare this to the quadratic-cost case. In that case, (i) we have a closed-form solution to the MINLP P_j , and (ii) the z_j^k are discrete convex (in k). It may be that even in the present more general case, possibly utilizing further technical assumptions, the z_j^k are discrete convex (as yet, we are unable to prove this). Regardless, we can compute the lower convex envelope of the graph of z_j^k versus $k = \sum_{i \in M} y_i$ to derive the relevant inequalities. In this way, we do not have a closed form expression for the inequalities, but we can easily compute them.

References

[1] P. Bonami, A. Wächter, L.T. Biegler, A.R. Conn, G. Cornuéjols, I.E. Grossmann, C.D. Laird, J. Lee, A. Lodi, F. Margot and N. Sawaya, An algorithmic framework for convex mixed integer nonlinear programs. IBM Research Report RC23771, October 2005.

[2] P. Bonami and J. Lee, `Bonmin` Users' Manual, July 2006.

[3] Bonmin, `projects.coin-or.org/Bonmin`

[4] M. Duran and I.E. Grossmann. An outer-approximation algorithm for a class of mixed-integer nonlinear programs. *Mathematical Programming*, 36:307–339, 1986.

[5] R. Fourer, D. Gay and B. Kernighan, AMPL: A Modeling Language for Mathematical Programming, 2003.

[6] M.T. Hajiaghayi, M. Mahdian and V.S. Mirrokni, The facility location problem with general cost functions. Networks 42 (2003), no. 1, 42–47.

[7] Ipopt, `projects.coin-or.org/Ipopt`

[8] J. Lee, Mixed Integer Nonlinear Programming: Some Modeling and Solution Issues, 2006. To appear in the *IBM Journal of Research and Development*.

[9] J. Lee and W.D. Morris, Jr., Geometric comparison of combinatorial polytopes. Discrete Applied Mathematics, 55(2):163–182, 1994.

[10] M. Mahdian and M. Pál, Universal facility location. Algorithms—ESA 2003, 409–421, Lecture Notes in Comput. Sci., 2832, Springer, Berlin, 2003.

[11] P. Mirchandani and R. Jagannathan, Discrete facility location with nonlinear diseconomies in fixed costs. Facility location analysis: theory and applications (Namur, 1987). Ann. Oper. Res. 18 (1989), no. 1-4, 213–224.

[12] W. Murray and U.V. Shanbhag, A local relaxation method for nonlinear facility location problems. Multiscale optimization methods and applications, 173–204, Nonconvex Optim. Appl., 82, Springer, New York, 2006.

[13] G.L. Nemhauser and L.A. Wolsey, Integer and Combinatorial Optimization, John Wiley & Sons, 1988.

[14] M.S. Daskin, C.R. Coullard and L. Ozsen, Capacitated Facility Location Model with Risk Pooling, IE&MS Working Paper 03-014, Northwestern University, August 2003.

[15] D.R. Shier and P.M. Dearing, Optimal locations for a class of nonlinear, single-facility location problems on a network. Oper. Res. 31 (1983), no. 2, 292–303.

[16] L.-Y. Wu, X.-S. Zhang, and J.-L. Zhang, Capacitated facility location problem with general setup cost. Comput. Oper. Res. 33 (2006), no. 5, 1226–1241.