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Alternate approximation of concave cost functions for process design and supply chain optimization problems

Diego C. Cafaro[a,*], Ignacio E. Grossmann[b]

[a] INTEC (UNL – CONICET), Güemes 3450, 3000 Santa Fe, Argentina
[b] Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, USA

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ABSTRACT

This short note presents an alternate approximation of concave cost functions used to reflect economies of scale in process design and supply chain optimization problems. To approximate the original concave function, we propose a logarithmic function that is exact and has bounded gradients at zero values in contrast to other approximation schemes. We illustrate the application and advantages of the proposed approximation.

1. Introduction

For preliminary calculations in chemical process design and supply chain strategic planning problems, the equipment or facility cost ($f(x)$) increases non-linearly with the size or capacity (x), as a concave function (Biegler, Grossmann, & Westerberg, 1997; Ciric & Floudas, 1991; Szitkai et al., 2003). As a result, power law expressions of the form $f(x) = cx^r$ with exponents less than one are usually adopted for capturing the effects of economies of scale. In such optimization problems, one of the major decisions is whether or not to buy/construct a certain equipment/facility, as well as determining its size or capacity, x (Biegler & Grossmann, 2004). A major drawback of the typical concave cost function $f(x)$ is that its derivative at $x = 0$ (a feasible value for x) is unbounded, which causes failures in the Karush–Kuhn–Tucker conditions of the associated nonlinear program. Common methods for dealing with such difficulties are: (a) approximate the concave function by a piecewise linear function (Geoffrion, 1977), or (b) add a very small value ε to the variable x, thus slightly displacing the curve toward the negative values of x. Approximation (a) is computationally costly and rather imprecise unless a fine discretization of the domain is used. Although in principle approximation (b) is reasonable, it has a number of drawbacks, especially if the exponents are small. To overcome such limitations, an approximation of logarithmic form is proposed in this short note.

2. Concave cost function and classical approximation

Given is the concave cost function for economies of scale with the form: $f(x) = cx^r$, where variable $x \geq 0$ is the size of the equipment, $f(x)$ is the cost of the equipment of size x, $c > 0$ is a constant parameter, and $0 < r < 1$ is a real exponent. This function has the property that its derivative with respect to x becomes unbounded when $x = 0$. An approximation that has been used to avoid computational failures of Non-Linear Programming (NLP) and Mixed-Integer Non-Linear Programming (MINLP) solvers is to add a small value ε to the x in the function $f(x)$ (Ahmetović & Grossmann, 2011; Yee & Grossmann, 1990), so that: $f(x) \approx h(x) = c(x + \varepsilon)^r$. Although this approximation yields bounded derivatives at $x = 0$ and a relatively good estimation of $f(x)$ when small values of ε are adopted, it has several drawbacks:

1. The smaller the parameter ε, the more precise the estimation, but the larger its derivative at $x = 0$, since: $h'(x) = c(x + \varepsilon)^{r-1}$, and $h'(0) = c/\varepsilon^{1-r}$. If such derivatives become very large, NLP solvers can lead to failures since the Karush–Kuhn–Tucker conditions (Bazaraa, Sherali, & Shetty, 1994; Biegler, 2010) cannot be satisfied due to ill conditioning.
2. The function $h(x)$ at $x = 0$ is not exactly equal to zero but $h(x) = c\varepsilon^r$. If ε is not small enough, the decision "not to install", i.e. $x = 0$, may incur a non-negligible cost, particularly if r is small.

To illustrate some limitations with the approximation $h(x)$ with smaller values of r, consider the simple example presented in Fig. 1. There are $i = 1...8$ potential sites for locating one plant (denoted by "X"), and $j = 1...9$ markets (represented by "O"). The plant produces a single liquid product that is supplied by dedicated pipelines to

* Corresponding author. Tel.: +54 342 455 9175; fax: +54 342 455 0944.
E-mail address: dcafaro@fiq.unl.edu.ar (D.C. Cafaro).

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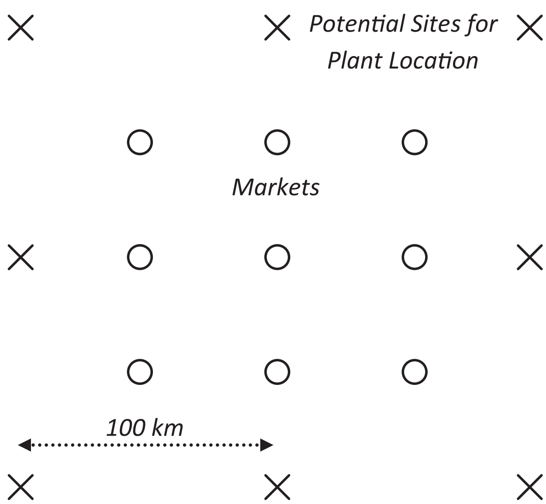

Fig. 1. An illustrative example.

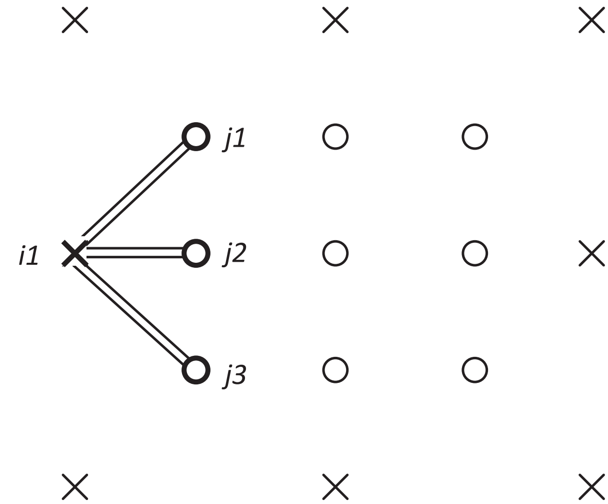

Fig. 2. Hypothetic solution for the example.

the selected markets. The plant capacity is given, and the fixed and variable charges for the plant installation (α_i, β_i) are independent on its location.

The aim of the problem is to determine the optimal location for the plant (denoted by the binary y_i) and the amount of product hourly supplied to every market ($q_{i,j}$), so as to maximize the annual benefits: $b(y_i, q_{i,j}) = \sum_{i,j}(pr_{i,j} - oc_{i,j})q_{i,j} - \sum_i(\alpha_i y_i + \beta_i \sum_j q_{i,j}) - z(q_{i,j})$ (sales income − operation costs − plant installation costs − pipeline costs). Since: (a) the product price and operation costs are independent of the plant location and markets supplied ($pr_{i,j} = pr$; $oc_{i,j} = oc$ $\forall i,j$), (b) only one plant will be selected ($\sum_i y_i = 1$), (c) the plant capacity Cap, is given ($\sum_{i,j} q_{i,j} = Cap$), and (d) fixed and variable costs for the plant installation are independent of the location ($\alpha_i = \alpha$; $\beta_i = \beta$ $\forall i$), it yields $b(y_i, q_{i,j}) = (pr - oc)\,Cap - \alpha - \beta\,Cap - z(q_{i,j})$, and the only variable terms in the objective function are pipeline costs $z(q_{i,j})$.

The pipeline flow (equal to the variable $q_{i,j}$) is proportional to the pipeline section, i.e. $q_{i,j} = K_1 d_{i,j}^2$, where d (m) is the pipeline diameter and K_1 has a value of 4239 m/h ($\pi/4 \times 3600$ s/h $\times$ 1.5 m/s). For simplicity, pipeline diameters are treated as continuous variables. Pipeline installation costs follow an economy of scale function of the form: $z(L_{i,j}, d_{i,j}) = K_2 L_{i,j} d_{i,j}^{0.60}$, where $L_{i,j}$ (km) is the distance between i and j (a given parameter) and K_2 = 1,132,500$ km^{-1} m$^{-0.60}$. Thus, the MINLP model is as follows:

$$
\begin{aligned}
& Min\, z = \sum_{i \in I, j \in J} K_2 L_{i,j} d_{i,j}^{0.60} \\
& S.t. \sum_{j \in J} q_{i,j} = Cap\, y_i \quad \forall i \in I \\
& \sum_{i \in I} y_i = 1 \quad q_{i,j} = K_1 d_{i,j}^2 \quad \forall i \in I, j \in J \quad q_{i,j} \le Dem_j \quad \forall i \in I, j \in J \\
& q_{i,j}, d_{i,j} \ge 0 \quad y_i \in \{0, 1\}
\end{aligned}
\tag{1}
$$

By substituting for $d_{i,j}$ in the objective function with the pipeline flow equation in the constraints, i.e. $d_{i,j} = (q_{i,j}/K_1)^{0.50}$, we obtain:

$$
\begin{aligned}
& Min\, z = \sum_{i \in I, j \in J} f(q_{i,j}) = \sum_{i \in I, j \in J} (K_2/K_1^{0.30}) L_{i,j} q_{i,j}^{0.30} \\
& S.t. \sum_{j \in J} q_{i,j} = Cap\ y_i \quad \forall i \in I \\
& \sum_{i \in I} y_i = 1 \quad q_{i,j} \le Dem_j \quad \forall i \in I, j \in J \\
& 0 \le q_{i,j}, \quad y_i \in \{0, 1\}
\end{aligned}
\tag{2}
$$

Note that the exponents of $q_{i,j}$ in the non-linear terms of the objective function are only 0.30.

Assume that the optimal solution is the one depicted in Fig. 2, where $y_{i1} = 1$, $q_{i1,j} = 175$ m^3/h for $j = j1, j2, j3$; $d_{i1,j} = 0.2032$ m (8 inches) for $j = j1, j2, j3$; while all the other variables take a zero value. Using the ε-approximation of $f(q_{i,j})$ with a reasonable value for $\varepsilon = 0.01$, the cost of the selected pipelines will be: $h(q_{i1,j1}) = h(q_{i1,j3}) = 92{,}440 \times 70.71 \times (175 + 0.01)^{0.30} = 30.77936$ MM$; $h(q_{i1,j2}) = 92{,}440 \times 50 \times (175 + 0.01)^{0.30} = 21.76451$ MM$; which is quite close to the actual values: $f(q_{i1,j1}) = f(q_{i1,j3}) = 92{,}440 \times 70.71 \times 175^{0.30} = 30.77884$ MM$; $f(q_{i1,j2}) = 92{,}440 \times 50 \times 175^{0.30} = 21.76413$ MM$.

However, for all the non-selected pipelines featuring $q_{i,j} = 0$ (totaling 69 non-used arcs $i - j$) the approximate installation cost is $h(q_{i,j}) = h(0) = 92{,}440\, L_{i,j}\ (0 + 0.01)^{0.30} = 23{,}220\, L_{i,j}$. Summing the lengths of the non-selected pipelines (9032 km) yields a total of 209.72194 MM$ instead of zero! In fact, the total pipeline cost in the optimal solution is $\sum_{i,j} f(q_{i,j}) = 83.32181$ MM$, while the approximation with $\varepsilon = 0.01$ results in the incorrect value of $\sum_{i,j} h(q_{i,j}) = 2 \times 30.77936 + 21.76451 + 209.71906 = 293.04517$ (252% error!). If we try a very small value for ε, say $\varepsilon = 10^{-9}$, this results in $\sum_{i,j} h(q_{i,j}) = 84.98768$ (2% error). However, the derivatives of every term $h(q_{i,j})$ at $q_{i,j} = 0$ increase to $h'(0) = 1.844 \times 10^{11} L_{i,j}$ (over 9.220×10^{12}), i.e. an unacceptably large value for NLP solvers. The new approximation proposed in the next section is intended to overcome such limitations, especially for concave cost functions with $r < 0.5$.

3. Logarithmic approximation of the concave cost function

We propose the following approximation function $g(x)$ for $f(x)$: $f(x) = cx^r \approx g(x) = k \ln(bx + 1)$, where x is the size of the equipment, $f(x)$ is the actual cost of the equipment of size x, $g(x)$ is the estimated cost, and k, $b > 0$ are real numbers selected to fit $f(x)$ as closely as possible. The proposed function has two main advantages:

1. The cost of $x = 0$ is exactly zero: $g(0) = k \ln(b0 + 1) = k \ln(1) = 0$.
2. The derivatives of $g(x)$ for all $x \ge 0$ are positive (bounded) values, given by $g'(x) = bk/(bx + 1)$. In particular at the origin ($x = 0$), $g'(x) = bk$.