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Alternate Approximation of Concave Cost Functions for Process Design and Supply Chain Optimization Problems

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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 (Ciric and Floudas, 1991; Biegler et al., 1997; Szitkai et al., 2003). As a result, power law expressions of the form $f(x) = c\, x^r$ 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 and 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),

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or (b) add a very small value ε to the variable x, thus slightly displacing the curve towards 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: $f(x) = c\, x^r$, 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 $f(x)$ (Yee and Grossmann, 1990; Ahmetović and Grossmann, 2011), 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 (Bazaara et al., 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 Figure 1. There are $i = 1\ldots8$ potential sites for locating one plant (denoted by "X"), and $j = 1\ldots9$ markets (represented by "O"). The plant produces a single liquid product that is supplied by dedicated pipelines to 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.

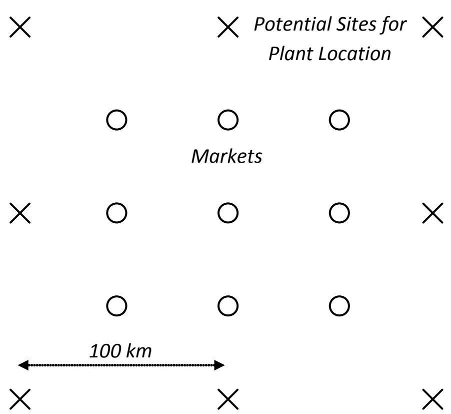

Figure 1. *An illustrative example*

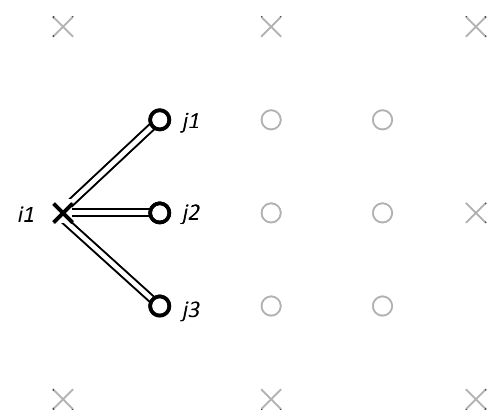

Figure 2. *Hypothetic solution for the example*

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 ($pr_{i,j} = pr$; $oc_{i,j} = oc \quad \forall i,j$), (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 ($\alpha_i = \alpha$; $\beta_i = \beta \quad \forall i$), 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 4,239 m/h (π / 4 × 3600 s/h × 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:

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

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:

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

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 Figure 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 (9,032 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 $h'(0) = 1.844\ 10^{11}\ L_{i,j}$ (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 $f(x)$: $f(x) = c\, x^r \approx g(x) = k \ln(bx + 1)$, 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: $g(0) = k \ln(b\, 0 + 1) = k \ln(1) = 0$.
2. The derivatives of $g(x)$ for all $x \geq 0$ are positive (bounded) values, given by $g'(x) = bk / (bx + 1)$. In particular at the origin ($x = 0$), $g'(x) = bk$.

In order to find appropriate values for b and k, a simple approach is to select two non-zero values for the variable x ($0 < x_1 < x_2$) and solve the following system of non-linear equations:

$$\left.\begin{aligned} c\, x_1^{\,r} &= k \ln(b x_1 + 1) \\ c\, x_2^{\,r} &= k \ln(b x_2 + 1) \end{aligned}\right\} \tag{3}$$

where k and b are the two values to be determined. Since $c, r, x_1, x_2 > 0$, we can divide both expressions to obtain: $(x_1 / x_2)^r = \ln(bx_1 + 1) / \ln(bx_2 + 1)$, which in turn can be rearranged as: $x_1^r \ln(bx_2 + 1) - x_2^r \ln(bx_2 + 1) = 0$. The implicit equation for variable b can be easily solved, for instance, using Newton's method, to find the value of b and by extension the value of k that satisfies: $f(x_1) = g(x_1)$ and $f(x_2) = g(x_2)$.

Let us reconsider the illustrative example, where $f(q_{i,j}) = 92{,}440\ L_{i,j}\ q_{i,j}^{0.30}$, with $0 \leq q_{i,j} \leq 525$. Since the first two factors are given, we analyze $\phi(q_{i,j}) = q_{i,j}^{\ 0.30}$, and following the procedure explained above, we can formulate the following system of equations:

$$\left.\begin{aligned} q_1^{\,0.30} &= k \ln(b q_1 + 1) \\ q_2^{\,0.30} &= k \ln(b q_2 + 1) \end{aligned}\right\} \tag{4}$$

Regarding the values of q_1 and q_2, we can make the selection based on our knowledge on the problem. Suppose that if a pipeline is installed, it is unlikely to supply less than $q_{lo} = 50$ m^3/h, while $q_{up} = 525$ m^3/h (the plant capacity) is the maximum possible flow. Then, we may simply set $q_1 = 50$ and $q_2 = 525$ to obtain: $b = 0.158815$; $k = 1.47613$, which leads to $\phi(q) = q^{0.30} \approx \gamma(q) = 1.47613 \ln(0.158815\, q + 1)$. Alternatively, less extreme values (for instance, $q_1 = 145$, $q_2 = 430$), may yield better approximations ($\gamma(q) = 1.64756 \ln(0.095853\, q + 1)$). Figure 3 shows the comparison of the two proposed approximations with the actual function, as well as the values of the derivatives at the origin, which in fact are rather small.

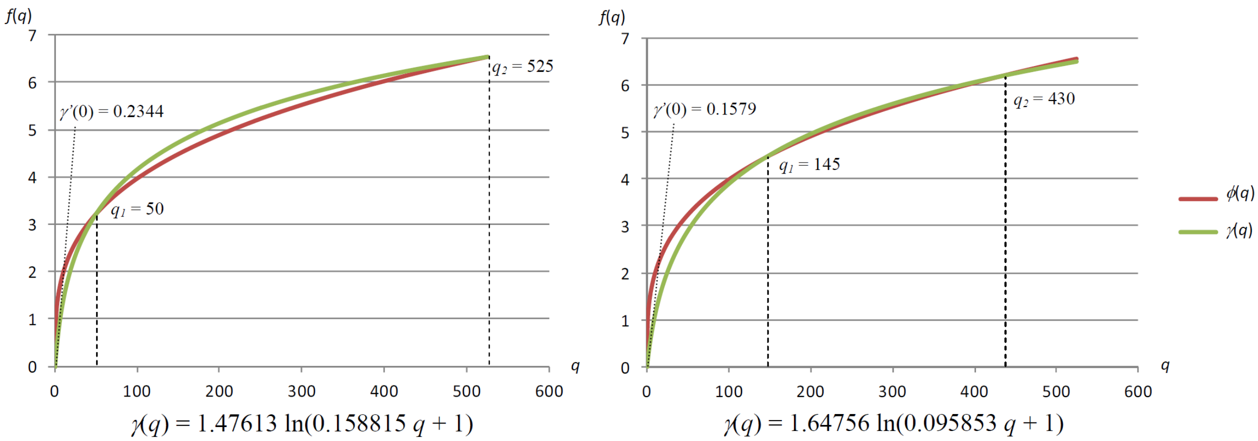

Figure 3. *Actual concave function (ϕ) and logarithmic approximations (γ)*

By determining the absolute and relative errors of the latter option (see Figure 4) it can be seen that close to the origin the estimations are not very accurate as expected, but in the origin the estimation is exact. Relative errors are below 2 % in the set $x \in \{0\} \cup [105\ ;\ 525]$.

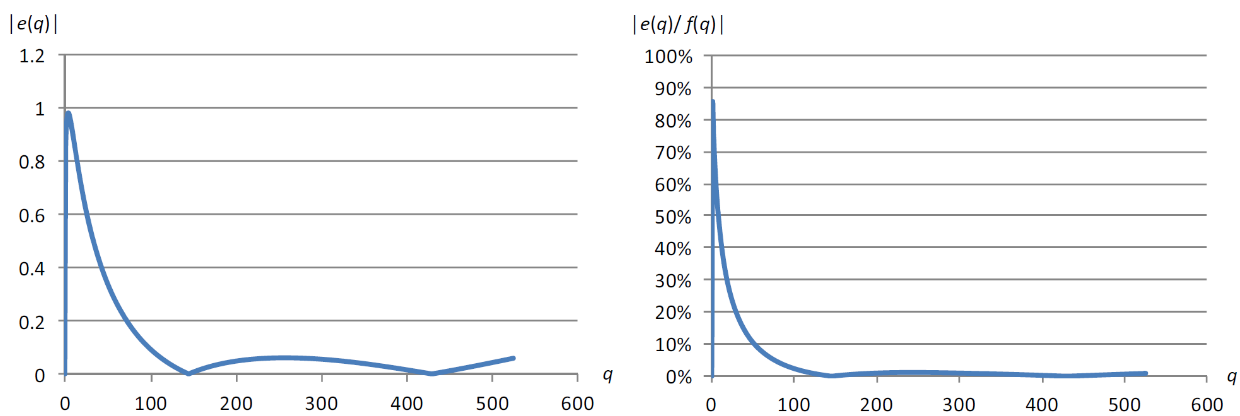

Figure 4. *Absolute and relative errors of the approximation* $\gamma(q) = 1.64756 \ln(0.095853\, q + 1)$

Revisiting the optimal solution assumed for the problem ($y_{i1} = 1$, $q_{i1,j} = 175$ m^3/h for $j = j1, j2, j3$; $d_{i1,j} = 0.2032$ m (8") for $j = j1, j2, j3$; and all the other variables with a zero value), the estimated cost of the selected pipelines is: $g(q_{i1,j1}) = g(q_{i1,j3}) = 92{,}440 \times 70.71 \times [1.64756 \times \ln(0.095853 \times 175 + 1)] =$ 30.99099 MM\$; $g(q_{i1,j2}) = 92{,}440 \times 50 \times [1.64756 \times \ln(0.095853 \times 175 + 1)] =$ 21.91415 MM\$; which is close to the actual values: $f(q_{i1,j1}) = f(q_{i1,j3})$ = 92,440 × 70.71 × $175^{0.30}$ = 30.77884 MM$; $f(q_{i1,j2})$ = 92,440 × 50 × $175^{0.30}$ = 21.76413 MM$ (only 0.6893 % error!).

Perhaps even more important, all the pipelines that are not selected ($q_{i,j} = 0$) feature the exact value of $g(q_{i,j}) = g(0) = f(0) = 0$. Therefore, the total pipeline installation cost ($\sum_{i,j} f(q_{i,j})$ = 83.32181 MM$) is very close to that one found through the proposed approximation, given by: $\sum_{i,j} g(q_{i,j})$ = 2 × 30.99099 + 21.91415 = 83.89613 MM$ (0.6893 % error).

Other approaches for parameter estimation

Another approach for estimating parameters k and b in the proposed function $g(x) = k \ln(bx + 1)$ is to consider a set of n representative values for variable x ($x_1, x_2, \ldots, x_n$) together with the actual values of the function $f(x)$ at that points ($f_1, f_2, \ldots, f_n$) and solve a least squares NLP problem of the form:

$$\begin{aligned} &\underset{k,b}{Min} \quad z = \sum_{i=1}^{n} (g_i - f_i)^2 \\ &S.t. \quad g_i = k \ln(b\, x_i + 1) \quad \forall i = 1 \ldots n \end{aligned} \tag{5}$$

Note that the values of the function $f(x)$ at the reference points can be obtained either from the original expression $f(x) = c\, x^r$, or from the real-world costs of equipments of size x.

For the illustrative example, we propose the representative values for q and $\phi(q)$ presented in Table 1. The NLP model proposed in (5) is solved to global optimality in 0.16 CPU s and 25 iterations using GAMS/BARON 9.0.6 (in an AMD Phenom Dual Core Processor at 2.90 GHz), setting 0 and 100 as lower and upper bounds for k and b. The optimal results yield b = 0.142310; k = 1.48658, with the total sum of square errors equal to 0.059, and the error distribution shown in Table 1. By minimizing the squared errors, the approximate function matches the actual function at lower values (q = 75). In this way, the error at q_{lo} = 50 is bounded more tightly.

Table 1. Representative values for q and $\phi(q)$, and approximation errors of $\gamma(q)$ using least squares

q	50	150	250	350	450	525
$\phi(q) = q^{0.30}$	3.23364	4.49601	5.24061	5.79723	6.25121	6.54708
$e = \gamma(q) - \phi(q)$	-0.121	0.122	0.110	0.042	-0.045	-0.115

Alternatively, model (5) can be solved using 1-norm for the deviations between the approximate and the actual values. This leads to b = 0.092164; k = 1.66748, yielding the best approximation for the original problem with a total error of 0.51 % in the pipeline costs.

4. COMPUTATIONAL RESULTS

The proposed approximation has been implemented in the objective function of an MINLP model for optimizing the design and development of the shale gas supply chain (Cafaro and Grossmann, 2013) with very promising results, particularly when applied to the estimation of gas and liquid pipeline costs, whose economies of scale exponents (with regards to the fluid flows) are typically 0.225 and 0.300, respectively. Very good results are also obtained in MINLP models of chemical process design problems, like the heat exchanger network synthesis (Yee and Grossmann, 1990) and the optimal design of process water networks (Ahmetović and Grossmann, 2011). In both cases, economies of scale functions with larger exponents (0.60 - 0.70) are effectively handled, always finding the optimal solution in short CPU times. In fact, the proposed approximation differs less than 0.70 % from the actual equipment costs.

In particular, the heat exchanger network synthesis problem, SYNHEAT, contributed by T. F. Yee to the GAMS model library (McCarl, 2011) is studied. By assuming that the exponent "*aexp*" is equal to 0.60 and implementing the proposed logarithmic approximation, the global optimum is found in 0.227 CPUs by solving GAMS/DICOPT2x-C. On the contrary, when applying the ε-approximation with $\varepsilon = 10^{-6}$, DICOPT can only find a suboptimal solution that is 6.8 % worse, starting from the same initial point given by default (see Table 2). If the value of ε is increased to 10^{-2}, an improved suboptimal solution is found, and the CPU time increases by a factor of 2.

When no approximation in the objective function is implemented and the outer-approximation algorithm (DICOPT) is used, the optimal solutions of the MILP steps in iterations 1 and 2 are $3.3\ 10^{13}$ and $6.3\ 10^{13}$, respectively. These are very large numbers that reflect the unbounded gradients of exchangers with zero size. By chance, even under these circumstances, the MILP model finds an integer solution that is solved in the NLP step yielding a value that is exactly the global optimum. However, it can be concluded that using directly the concave functions in the algorithm is not reliable. On the other hand, from Table 2 we can see that with the proposed logarithmic approximation values within 0.60 % of the global optimum are found with DICOPT and BARON.

Table 2. Computational results for the heat exchanger network synthesis problem (SYNHEAT)

	MINLP Solver	Approximate Solution	Actual Solution	Approximation Error	Deviation from the Optimum	CPUs
no-approx	DICOPT	110,170	110,170	0 %	0 %	0.272
	BARON	110,170	110,170	0 %	0 %	348.61
ε-approx $\varepsilon = 10^{-6}$	DICOPT	117,629	117,629	$2.6\ 10^{-4}$ %	6.8 %	0.296
	BARON	110,170	110,170	$3.1\ 10^{-4}$ %	0 %	30.68
ε-approx $\varepsilon = 10^{-2}$	DICOPT	115,757	115,670	0.08 %	5.0 %	0.521
	BARON	110,257	110,170	0.08 %	0 %	71.68
log-approx	DICOPT	109,531	110,170	0.58 %	0 %	0.227
	BARON	109,531	110,170	0.58 %	0 %	77.07

5. CONCLUSIONS

An alternate approximation of concave cost functions that captures economies of scale in process design and supply chain optimization problems has been presented. The proposed logarithmic expression is very simple, fits quite well to the original power law functions, and overcomes the drawbacks of large derivatives and large estimation errors that are experienced with small exponents using approximations that add the tolerance ε. Promising results are obtained when applying the approach to well-known process design problems and real-size case studies related to the strategic planning of natural gas supply chains. The proposed approximation is particularly useful when large superstructures and low exponents (as for pipeline costs) are considered.

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