

# Bridging the Gap Between Heuristics and Optimization: Capacity Expansion Case

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*The competition between heuristic and optimization approaches for process synthesis and process operations problems has caused major controversy in recent years. Heuristics offer fast solutions but no guarantee of optimality. Mathematical programming approaches, on the other hand, offer rigor but suffer from combinatorial explosion of computational requirements. The use of analytical investigations is proposed as a theoretical means to characterize the behavior of heuristics and optimization algorithms and produce a framework that combines the strengths of the two approaches while eliminating their weaknesses. The approach contrasts and complements the current practice in process systems engineering, which is entirely empirical in nature. The proposed paradigm is demonstrated in the context of the multiperiod capacity expansion problem for chemical process networks, a problem having much in common with both process synthesis and operations problems. Analytical investigations for this problem lead to the development of a heuristic that is proved to be asymptotically optimal under standard assumptions about the problem parameters. In the more general context of process synthesis and operations, analytical investigations present a large array of opportunities.*

## Introduction

The combinatorial nature of problems in process systems engineering has long been recognized and, over the last couple of decades, has led naturally to the establishment of mixed-integer optimization techniques as a major paradigm. This is evidenced by the many integer programming approaches to problems spanning the range including process design and process synthesis as well as process planning and scheduling (Grossmann, 1985, 1989, 1996; Grossmann and Daichendt, 1994; Reklaitis, 1989, 1992).

Despite the success of optimization models and algorithms in solving problems of industrial relevance, the majority of approaches in current industrial-level design practice are still based on *heuristic* rather than integer programming techniques. The major argument against using the optimization approach is that the number of problems that can be solved to *global optimality* (or *exactly*) is limited, due to the combinatorial nature of these problems. The number of possible solutions and, thus, the number of worst-case iterations of exact

algorithms, increases exponentially as the size of the problem increases. On the other hand, heuristics developed for synthesis, design, and operations of chemical processes lack the rigor of optimization methods, as they are not guaranteed to provide near-optimal or even feasible solutions. Evidently, the competition between heuristic and optimization approaches has led to a major controversy, as members of the process systems engineering community in industry and academia have been polarized toward one or the other approach (Stephanopoulos, 1980).

Recognizing the current gap between heuristic and optimization approaches in process systems engineering, we ask:

- Is it possible to introduce rigor in the use and practice of heuristics?
- Is it possible to solve combinatorial optimization problems in an approximate way that escapes the curse of dimensionality without a significant compromise of optimality?

This article proposes the use of *analytical investigations*, namely, worst-case analysis and probabilistic analysis, to bridge the gap between heuristics and exact algorithms in

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process systems engineering. *Worst-case analysis* bounds the maximum amount that a heuristic solution will deviate from optimality for any problem. Although useful in understanding when and why the heuristic will perform its worst, in practice this type of analysis is usually not predictive of average performance. On the other hand, *probabilistic analysis* provides mathematical expressions for the probable (*expected*) behavior of heuristics. Ideally, one would like to solve a difficult problem using a heuristic whose behavior is probably near optimal. This approach combines the speed of heuristics with the solution quality of optimal approaches.

Modern computational theory recognizes analytical investigations as a distinct subject (Karp et al., 1985; Fisher, 1980). Nevertheless, because they are usually very tedious and far from trivial, analytical studies of algorithms form a very fragmented literature of mostly problem-specific results. Furthermore, the ideas regarding the analytical development of properties of algorithms are not known to obey any unifying theory; there are no recipes to follow in order to analytically investigate a new problem.

To demonstrate the potential of analytical investigations, this article develops such an approach for the problem of designing a network of interconnected chemical processes (batch and/or continuous, flexible and/or dedicated) in a way that maximizes the operations' net present value over a given time horizon. This capacity-expansion problem has in the past been approached through models that discretize the time horizon into a finite number of time periods. Solution algorithms have been developed based on integer programming (Sahinidis et al., 1989; Sahinidis and Grossmann, 1992; Liu and Sahinidis, 1995, 1996) and continuous global optimization (Liu et al., 1996). The reason for selecting this problem as the test bed of the proposed ideas is because it has much in common with both process operations and process synthesis problems. Indeed, multiperiod capacity expansion shares many of the characteristics of multiperiod process scheduling when both problems are viewed through a time discretization framework (Sahinidis and Grossmann, 1991). At the same time, the problem requires the design of a network by extracting the optimal solution from a superstructure, much like in most synthesis problems (Nishida et al., 1981).

A review of the literature of analytical approaches is provided in the next section, whereas the subsection on problem description reviews the capacity expansion problem. In the subsections titled "Theoretical Analysis of Linear Relaxation" and "Theoretical Analysis of an Optimization-based Heuristic" we present worst-case and probabilistic analyses to *prove* a number of properties for this process design/operational problem. The main results are that, as the number of time periods and, thus, the combinatorial difficulty of the problem, increases:

- The linear programming relaxation gap of the corresponding integer programming formulation does not worsen. For problems with an infinite time horizon, this gap vanishes with "probability one."

- A simple linear programming-based heuristic provides optimal solutions for large-scale problems "almost surely."

Computational results presented in the subsection on empirical analysis verify the theoretical predictions.

By studying the set of optimal solutions to the corresponding integer program, we conclude that an optimization-based

heuristic approach provides provably optimal solutions for large-scale instances of the problem considered in the article. It is expected that similar analytical approaches will provide very useful insight to other process synthesis and operational problems. The main conclusion of the "Conclusions" section is that analytical investigations of exact and heuristic algorithms are needed to complement the current empirical investigations of problems in process systems engineering.

## Analysis of Algorithms

In the analysis of algorithms it is customary to classify problem-solving procedures based on how their running time increases as a function of problem size (see Garey and Johnson, 1991; Papadimitriou, 1994). In one such classification, algorithms whose running time can be bounded from above by a polynomial function of the input size are considered to be "good," whereas algorithms whose running time cannot be so bounded are considered to be "bad." Problems for which polynomial algorithms exist are said to belong to the complexity class  $\mathcal{P}$ . This class is a subset of the more general class  $\mathcal{NP}$  that includes problems for which *verification* of a candidate solution can be done in polynomial time. However, there are some problems in  $\mathcal{NP}$  for which no polynomial *solution* algorithm currently exists. These problems might require an exorbitant amount of time to be solved on conventional computers. The theory of polynomial time reducibility and  $\mathcal{NP}$ -completeness (Cook, 1971) establishes the equivalence between the hardest of all problems in  $\mathcal{NP}$ , the so-called  $\mathcal{NP}$ -complete problems. If any one of these problems can be solved polynomially, they all can, implying that  $\mathcal{P} = \mathcal{NP}$ . However, it is widely believed that polynomial algorithms for  $\mathcal{NP}$ -complete problems do not exist.

Solving optimization problems with linear objectives and constraints is a problem in  $\mathcal{P}$ . On the other hand, most problems requiring the solution of integer programs are known to be  $\mathcal{NP}$ -complete. Most engineering design problems belong to this class. The absence of fast algorithms for these difficult problems naturally prompts the development of approximate algorithms (heuristics). These are fast (polynomial) algorithms that, however, offer no guarantee of optimality.

It should be emphasized that the classification into  $\mathcal{P}$  and  $\mathcal{NP}$ -complete is based on worst-case analysis. In other words, if any single instance of a problem requires superpolynomial resources to be solved, the problem cannot be classified in  $\mathcal{P}$ . It is therefore obvious that such classifications might turn out to be overly pessimistic and unrealistic for many engineering problems. From a practical point of view, with many problem instances awaiting solution, the *average* behavior of an algorithm is a more realistic performance measure. Simply stated, for  $\mathcal{NP}$ -complete problems, algorithm designers would like to discover polynomial time algorithms that, while not guaranteed to always find optimal solutions, are expected with high probability to produce solutions that are close to optimal.

Probabilistic analysis of algorithms characterizes the expected behavior of algorithms. The origins of this concept can be traced back to an article by Beardwood et al. (1959) dealing with special cases of the traveling salesman problem. However, it was not until after Cook's 1971 work on  $\mathcal{NP}$ -completeness that Karp (1976) demonstrated the potential

importance of probabilistic analysis in a number of combinatorial search algorithms. Following these developments, we have witnessed three types of probabilistic analysis, namely, probabilistic running time analysis, probabilistic error analysis, and probabilistic value analysis, dealing, respectively, with the running time of algorithms, the deviation of a heuristic solution from the optimum, and the optimal solution value in terms of the problem parameters. The analysis is typically confined to classical combinatorial problems such as the knapsack problem, the bin-packing problem, facility-location problems, vehicle-routing and traveling salesman problems, and certain scheduling problems. A review of this topic appears in Karp et al. (1985).

In addition to probabilistic analysis, two more avenues can be taken when studying exact and heuristic algorithms. *Empirical analysis* is the actual computational testing of algorithms and is the most frequently taken approach. *Worst-case analysis* provides bounds on the worst possible deviation of the heuristic solution from the optimum. Ideally, one would like to design heuristics that are fast and deterministically guaranteed to produce near-optimal results. The results in the relevant body of the literature are quite specialized and no unifying theory yet exists (Fisher, 1980).

The advantages and disadvantages of the three different paradigms in the study of heuristics should be clear. Empirical analysis is computationally very expensive and offers no guarantee on the heuristic's performance on problems other than the ones solved. Worst-case analysis corrects this deficiency by showing the worst possible deviation of a heuristic from the optimum. However, it is not predictive of average performance. Probabilistic analysis, on the other hand, fills the void between empirical and worst-case analysis as it shows how the algorithm will perform in a "typical" problem instance. Its main disadvantage is that it requires assumptions on the probability distributions of the problem data. In addition, results of probabilistic analysis might be only asymptotic, that is, valid for very large-scale problems. In this case, empirical analysis is required to investigate whether the results of probabilistic analysis are meaningful for smaller problem sizes. Clearly, empirical, probabilistic, and worst-case analysis complement one another. The main advantage of the latter two is that they require algorithm developers to understand how their algorithms will perform in the average or worst case. Thus, analytical investigators foster new insights into algorithmic and problem structure.

Previous work in process systems engineering has focused exclusively on empirical analysis of algorithms. For the problem studied in the following section, we present worst-case as well as probabilistic analyses. As the probabilistic results are asymptotic, we also present empirical evidence demonstrating that these results are valid for realistic problem sizes.

## Analysis of Multiperiod Design and Operation of Chemical Process Networks

### Problem description

We consider the problem of long-range capacity expansion and operational decisions for a chemical process complex. The complex involves a number of processes interconnected by raw materials, intermediates, and products. Products may be purchased from and/or sold to different markets. The deci-

sion problem requires (i) selecting processes from among competing technologies, (ii) timing process expansions, (iii) determining the optimal production levels for the installed processes. The design objective is to maximize the net present value for the entire complex over a long-range horizon. The time horizon consists of a number of time periods during which prices and demands of chemicals, and investment and operating costs of the processes can vary.

Assuming linear mass balances, linear operating costs, and investment costs with economies of scale, the problem can be formulated as an integer program following closely Sahinidis et al. (1989):

### Model P

$$\max z = \sum_{j=1}^C \sum_{l=1}^M \sum_{t=1}^n (\gamma_{jlt} S_{jlt} - \Gamma_{jlt} P_{jlt}) - \sum_{i=1}^N \sum_{t=1}^n (\alpha_{it} X_{it} + \beta_{it} y_{it} + \delta_{it} W_{it}), \quad (1)$$

subject to

$$0 \leq X_{it} \leq y_{it} X_i^U \quad i = 1, \dots, N; \quad t = 1, \dots, n \quad (2)$$

$$Q_{it} = Q_{i,t-1} + X_{it} \quad i = 1, \dots, N; \quad t = 1, \dots, n \quad (3)$$

$$W_{it} \leq \tau_t Q_{it} \quad i = 1, \dots, N; \quad t = 1, \dots, n \quad (4)$$

$$\sum_{l=1}^M P_{jlt} + \sum_{i=1}^N \eta_{ij} W_{it} = \sum_{l=1}^M S_{jlt} + \sum_{i=1}^N \mu_{ij} W_{it} \quad j = 1, \dots, C; \quad t = 1, \dots, n \quad (5)$$

$$a_{jlt}^L \leq P_{jlt} \leq a_{jlt}^U \quad j = 1, \dots, C; \quad l = 1, \dots, M; \quad t = 1, \dots, n \quad (6)$$

$$d_{jlt}^L \leq S_{jlt} \leq d_{jlt}^U \quad j = 1, \dots, C; \quad l = 1, \dots, M; \quad t = 1, \dots, n \quad (7)$$

$$Q_{it}, W_{it}, P_{jlt}, S_{jlt} \geq 0 \quad \forall i, j, l, t \quad (8)$$

$$y_{it} = 0 \text{ or } 1 \quad i = 1, \dots, N; \quad t = 1, \dots, n. \quad (9)$$

The indices  $i$ ,  $j$ ,  $l$ , and  $t$  in the preceding equations denote processes ( $i = 1, \dots, N$ ), chemicals ( $j = 1, \dots, C$ ), markets ( $l = 1, \dots, M$ ), and time periods ( $t = 1, \dots, n$ ), respectively; and  $N$ ,  $C$ ,  $M$ , and  $n$ , respectively, denote the number of processes, number of chemicals, number of markets, and number of time periods of the problem.

The integer decision variable,  $y_{it}$ , is 1 whenever there is an expansion for process  $i$  at the beginning of time period  $t$ , and 0 otherwise. The continuous problem variables are capacity expansions ( $X_{it}$ ), capacities ( $Q_{it}$ ) and operating levels ( $W_{it}$ ) for processes, and purchase ( $P_{jlt}$ ) and sales amounts ( $S_{jlt}$ ) for chemicals.

The given parameters for this formulation are bounds for chemical availabilities ( $a_{jlt}$ ) and demands ( $d_{jlt}$ ), existing capacities ( $Q_{i0}$ ), bounds on capacity expansions ( $X_i^U$ ), stoichiometric coefficients for mass balances ( $\eta_{ij}$ ,  $\mu_{ij}$ ), variable investment costs ( $\alpha_{it}$ ), fixed investment costs ( $\beta_{it}$ ), sales prices

( $\gamma_{jit}$ ) and purchase prices ( $\Gamma_{jit}$ ) for chemicals, process operating costs ( $\delta_{it}$ ), and the lengths of time periods ( $\tau_i$ ). The time dependency of  $X_i^u$  is omitted for simplicity of presentation.

In Eq. 1,  $z$  is defined as the difference between the sales revenue and the sum of raw material costs, and investment and operating costs. Bounds for capacity expansions are enforced in Eq. 2 in accordance to the definition of the binary variables. Capacity expansions are added to previously installed capacities in Eq. 3 to provide the total capacity available for process  $i$  in period  $t$ . In Eq. 4, the operating level of a process is required not to exceed the corresponding installed capacity. For each chemical, purchases from various markets plus the amounts produced within the network must be equal to the sum of sales and the total consumption within the network. This requirement is expressed by the material balances for chemicals in constraint (Eq. 5). Finally, the simple constraints (Eqs. 6 and 7) express lower and upper bounds for raw material availabilities and product demands.

$P$  is a conventional planning model. The presence of the integer decision variables makes this model difficult to solve. A standard measure of solution difficulty of integer models is the relaxation gap, that is, the difference between the optimal solution value of the integer program and that of its linear programming relaxation. The next subsection develops analytical properties of the linear programming relaxation of  $P$ .

### Theoretical analysis of linear relaxation

The linear relaxation of  $P$  is obtained by replacing Eq. 9 by

$$0 \leq y_{it} \leq 1 \quad i = 1, \dots, N; \quad t = 1, \dots, n. \quad (10)$$

Let  $P_n$  denote a problem of the form of  $P$  with  $n$  time periods. We will use  $P_n^L$  to denote the linear programming relaxation of  $P_n$ . Also, let  $z_n$  and  $z_n^L$  be the optimal solution values of  $P_n$  and  $P_n^L$ , respectively. We are interested in studying the behavior of  $z_n^L - z_n$  as  $n$ , therefore the combinatorial difficulty of the problem, increases.

#### Worst-Case Analysis

**Theorem 1.** For any realization of coefficients of  $P_n$ , we have

$$z_n^L - N \times n \times \beta_{\max} \leq z_n \leq z_n^L,$$

where  $\beta_{\max} = \max_{i,t} \{\beta_{it}\}$ .

The mathematical proof of this and all theorems to follow can be found in the Appendix.

The interpretation of Theorem 1 is as follows. While the relaxation obviously provides an upper bound for  $z_n$ , at the same time, the solution of  $P_n^L$  can be rounded up to provide an integer solution that is feasible to  $P_n$ , and thus corresponds to a lower bound for  $z_n$ . In the worst case, all  $y$  variables will be fractional at the relaxed problem solution with values very close to zero. In this case, rounding of all  $y$  variables will change  $z_n^L$  by at most  $N \times n \times \beta_{\max}$ .

It is straightforward to extend the preceding and subsequent results to the case when nonzero lower bounds are included in Eq. 2. Theorem 1 provides an upper bound on the relaxation gap irrespectively of the problem data. It is therefore a worst-case result. Without any information on the so-

lution of the linear relaxation, the *a priori* bound of Theorem 1,  $\sum_{i=1}^N \sum_{t=1}^n \beta_{it}$ , for the relaxation gap is too loose. However, after solving the linear relaxation problem, we can get a tighter *posterior* bound, which is  $\sum_{(i,t) \in A} \beta_{it}(1 - y_{it}^*)$ , where  $A = \{(i,t): 0 < y_{it}^* < 1\}$ . Even then, the worst-case bound is still too loose as the next subsection shows.

**Probabilistic Analysis.** This subsection assumes familiarity with elementary definitions from probability and statistics (see, for example, Manoukian, 1986; Nguyen and Rogers, 1994). Central to the analysis to follow is the notion of convergence with probability one (w.p. 1) also known as convergence almost surely (a.s.), which is defined as follows:

**Definition 1.** Let  $A$  be an event of a probability space and  $Pr(A)$  denote its probability. If  $Pr(A) = 1$ , then  $A$  is said to occur almost surely. In particular, if, for a sequence of random variables  $\{x_n\}$ ,  $Pr(x_n \rightarrow x) = 1$ , then  $\{x_n\}$  converges to  $x$  a.s.

If the space of events is finite,  $Pr(A) = 1$  implies that event  $A$  is *certain*. If the space of events is infinite, a statement of the type "for problem  $P$ , condition  $A$  is true w.p. 1" implies that there might be some, yet finitely many, instances of problem  $P$  for which  $A$  is false, whereas there are infinitely many problem instances for which  $A$  is true.

To carry out probabilistic analysis, we will make the following assumptions regarding the problem data.

**Assumption 1.** All costs and prices are independent random variables with finite expectations. In particular, let  $\alpha = E(\alpha_{it})$ ,  $\forall i, t$ , and  $\beta = E(\beta_{it})$ ,  $i = 1, \dots, N$ ;  $t = 1, \dots, n$ .

**Assumption 2.** Demands and availabilities are independent random variables with bounded distributions.

**Assumption 3.** The fixed investment costs,  $\beta_{it}$ , are bounded:  $\beta_{it} \leq \beta^U$ ,  $i = 1, \dots, N$ ;  $t = 1, \dots, n$ .

We will provide a theoretical measure of the quality of the linear relaxation under two different modeling approaches:

- A fixed-length time-horizon problem with a growing number of time periods;
- A growing time-horizon problem.

The former case is of interest as finer time discretizations allow more accurate modeling of demand and price fluctuations. The latter case is of interest as it allows the modeling of problems with longer planning horizons.

**A. Fixed time horizon with infinite time periods.** We use the independent model approach for the sampling (drawing) of a series of problem instances of growing size  $n$  while  $N$ ,  $C$ , and  $M$  are fixed. Thus, each successive problem instance of size  $n+1$  is built up from the coefficients of the problem instance of size  $n$  by partitioning any one of the time periods, say period  $t$ , into two time periods of equal length. The coefficients of the new problem with size  $n+1$  are the same as in the problem of size  $n$  with the following exceptions. The costs and prices of the two newly introduced time periods are drawn randomly. Demands and availabilities of the two new time periods are obtained by splitting the demands and availabilities of time period  $t$  in half.

**Theorem 2.** Let  $K$  be the number of fractional components of  $y$  in an optimal solution of  $P_n^L$ . Then, there exists an optimal solution of  $P_{n+1}^L$  with  $K$  fractional components in  $y$  w.p. 1.

Since the planning horizon and product demands are finite, there is an upper bound on the maximum possible rev-

enues, which implies an upper bound on the maximum number of expansions in any profitable plan. Theorem 2 is, then, a consequence of the fact that, for sufficiently large  $n$ , the solution of the linear programming relaxation is likely to characterize all possible expansions; additional time periods are redundant to the representation of capacity expansions.

**Theorem 3.** Let  $K$  be the number of fractional components of  $y$  in an optimal solution of  $P_{n_0}^L$  for any number of time periods  $n_0$ . Then,

$$z_n^L - z_n \leq K \times \beta^U \quad \text{w.p. 1,} \quad \forall n > n_0.$$

This theorem is a corollary of Theorem 2. According to this result, the relaxation gap, for large  $n$ , is bounded by the number of processes  $\times$  the maximum possible fixed-charge cost. A consequence of this theorem is that, for a given capacity expansion problem with a fixed-length time horizon, finer discretizations do not worsen the quality of the linear programming relaxation. Therefore, finer discretization can be expected to not have a strong combinatorial effect on computational requirements.

**B. Infinite time horizon.** We use the independent model approach for the sampling of a series of problem instances of growing size  $n$  while  $N$ ,  $C$ , and  $M$  are fixed. Thus, each successive problem instance is built up by appending one new time period,  $n+1$ . Costs, prices, demands, and availabilities of time period  $n+1$  are all drawn randomly.

**Theorem 4.** There exists a number  $n_0$  such that  $\forall n > n_0$ , the solution of  $P_n^L$  has no more fractional components than the number of fractional components in the solution of  $P_{n_0}^L$  w.p. 1.

Qualitatively, the preceding theorem is true as, for sufficiently large  $n_0$ , the time period  $n_0$  will be generated with demands and availabilities corresponding to their expected extremal profitable values, thus necessitating the maximum possible capacity expansion to be installed by time period  $n_0$ . Therefore, additional time periods will not require any additional capacity expansions.

**Theorem 5**

$$\lim_{n \rightarrow \infty} \left( \frac{z_n^L}{n} - \frac{z_n}{n} \right) = 0 \quad \text{w.p. 1.}$$

According to this result, problems with a very large number of time periods can be expected to have no linear programming relaxation gap. Note that both  $z_n^L$  and  $z_n$  approach infinity as  $n \rightarrow \infty$ . The theorem states that their difference nevertheless remains finite. This clearly follows from Theorem 4, as, for sufficiently large  $n$ , no additional expansions are required and the relaxation solution does not worsen with the addition of time periods.

### Theoretical analysis of an optimization-based heuristic

The main observation in designing this heuristic is that the solution of the linear programming relaxation of the integer model satisfies all problem constraints except, possibly, for the integrality requirements (Eq. 9). Therefore, if we keep the operating profile (operating levels, purchase and sales amounts) as given in the relaxation solution and adjust the

capacity expansions and values of the binary decision variables in a way that satisfies integrality requirements, we will obtain a feasible solution to the integer program. One possibility is to simply round up those  $y_{it}$  variables that assumed noninteger values at the relaxed problem solution and keep all others at zero. However, such a simple-minded rounding scheme might result in a large number of capacity expansions and too much capital investment. To minimize the number of expansions, we will "shift" capacity from later to earlier time periods. To avoid unnecessary excess capacity, we will shift capacity only to time periods during which some capacity expansion is indicated in the relaxation solution. The details of the heuristic are as follows:

#### Algorithm 1. Heuristic

**Step 1.** Solve the linear programming relaxation. Let  $x^* = (X^*, Q^*, W^*, P^*, S^*, y^*)$  denote the solution of the relaxation. Set  $\bar{x} \leftarrow x^*$ .

**Step 2.** For all processes  $i \in \{1, \dots, N\}$ , find the indices  $t_i \in \{1, \dots, T\}$  such that  $y_{it}^* \neq 0$ . Let  $T_i = \{t_1, t_2, \dots, t_{p_i}\}$  denote such index sets for  $i \in \{1, \dots, N\}$ .

**Step 3.** For each process  $i \in \{1, \dots, N\}$ , set  $k \leftarrow 1$ , repeat Steps 3.1, 3.2, and 3.3 until  $k > p_i$ .

**Step 3.1.** Set  $h \leftarrow k$ .

Set  $\bar{y}_{it_h} \leftarrow 1$ .

Set  $k \leftarrow h+1$ .

**Step 3.2.** If  $\bar{X}_{it_h} + \bar{X}_{it_k} > X_i^U$ , go to Step 3.1.

If  $\bar{X}_{it_h} + \bar{X}_{it_k} \leq X_i^U$ , set  $\bar{X}_{it_h} \leftarrow \bar{X}_{it_h} + \bar{X}_{it_k}$ .

Set  $\bar{y}_{it_k} = 0$  and  $\bar{X}_{it_k} = 0$ .

**Step 3.3.** Set  $k \leftarrow k+1$ , go to Step 3.2.

**Step 4.** For each process  $i \in \{1, \dots, N\}$  and for  $t \in \{1, \dots, T\}$ , set  $\bar{Q}_{it} = \bar{Q}_{it-1} + \bar{X}_{it}$ .

The possibility of shifting the capacity expansion from  $t_h$  to the earlier  $t_k$  is exploited in Steps 3.1 and 3.2 of the algorithm. The rest of the algorithm is straightforward. Let  $z^H$  denote the objective value obtained from  $\bar{x}$ .

**Theorem 6.** The solution  $\bar{x}$  obtained by the preceding heuristic is feasible to  $P$  and  $z^H \leq z \leq z^L$ .

The worst-case behavior of the heuristic can be measured by comparing the heuristic value to that of the linear relaxation:

$$z^L - z^H = \sum_{i=1}^N \sum_{t \in T_i} (\alpha_{it} \bar{X}_{it} + \beta_{it} \bar{y}_{it}) - \sum_{i=1}^N \sum_{t \in T_i} (\alpha_{it} X_{it}^* + \beta_{it} y_{it}^*). \quad (11)$$

Since the components  $\bar{W}$ ,  $\bar{P}$ , and  $\bar{S}$  of  $\bar{x}$  are the same as that of  $x^*$ , Eq. 11 is easy to verify. Moreover, for each process  $i$ , only a small number of the  $\bar{y}_{it}$  and  $\bar{X}_{it}$  are nonzero. It can thus be expected that the difference  $z^L - z^H$  will be very small. We now turn our attention to a probabilistic analysis of the heuristic. We will use the two modeling approaches of infinite discretization and infinite time horizon used in the subsection on the infinite time horizon.

#### Fixed Time Horizon with Infinite Time Periods

##### Theorem 7

$$E(z_n^L - z_n^H) \leq N \times \beta.$$

Theorem 7 is obtained by taking expectations of both sides of Eq. 11 and recognizes the fact that the heuristic solution brings the relaxation solution closer to the integer optimum by shifting capacity to those earlier time periods in which expansion was allowed by the relaxed problem. The proof of this theorem (see Appendix) is very illuminating, as it clearly shows that the "simpleminded" heuristic of rounding up all the  $y_{it}$  variables does not share the strong optimality property of the rounding heuristic developed here, and thus produces suboptimal solutions.

#### Theorem 8

$$\lim_{n \rightarrow \infty} (z_n^L - z_n^H) \leq N \times \beta \quad \text{w.p. 1.}$$

This result is an obvious corollary of Theorem 7 and implies that the quality of the heuristic solution does not worsen as the number of time periods increases. Therefore, the behavior of the heuristic does not worsen as the combinatorial difficulty of the problem increases.

#### Infinite Time Horizon

#### Theorem 9

$$\lim_{n \rightarrow \infty} \left( \frac{z_n^L}{n} - \frac{z_n^H}{n} \right) = 0 \quad \text{w.p. 1.}$$

The importance of this theorem is that it shows that the heuristic can be expected to be optimal for problems with a very large number of time periods. This was expected in light of the earlier result that the relaxation gap vanishes for problems of this type.

### Empirical analysis

The previous subsections provided asymptotic results for the linear programming relaxation and the heuristic as the number of time periods  $n$  approaches infinity. Whether or not these asymptotic properties are valid for realistic problem sizes is the subject of the computational investigation of this subsection. We begin by solving a set of 23 problems from the existing literature. Subsequently, we report additional computational experience with the heuristic for randomly generated test problems with a variety of sizes, structures, and parameters. In all cases, the heuristic was implemented using the GAMS modeling system (Brooke et al., 1988) on a Sun SPARC station 2 and CPLEX (1993) was used to solve all the linear and integer programs.

Table 1 presents computational results from 23 test problems from Liu and Sahinidis (1995). Problems 8–23 are longer-horizon versions of problems 1–7. For each problem, we report the number of processes  $N$ , the number of time periods  $n$ , the number of 0–1 variables in the integer programming formulation, the value of the relaxation  $z^L$ , the exact solution value  $z$ , and the heuristic solution value  $z^H$ . The columns  $(z - z^L)/z \times 100$  and  $(z - z^H)/z \times 100$  list the percentage of relaxation gap and heuristic approximation error, respectively. Finally, the columns  $t_{IP}$  and  $t_H$  present the CPU requirements for solving the problems using integer programming and the heuristic, respectively. The table shows that 17 out of the 23 problems are solved optimally by the heuristic. Overall, the approximation error by the heuristic is only 0.5% on the average. At the same time, the average CPU requirements of the heuristic are less than 1 s, whereas two of these problems cannot be solved within 10 min with the

Table 1. Computational Results with Problems from the Literature

Problem	$N$	$n$	0-1	$z^L$	$z$	$z^H$	$(z - z^L)/z \times 100$	$(z - z^H)/z \times 100$	$t_{IP}$	$t_H$
1	3	3	9	1,898.1	1,774.8	1,774.8	6.9	0	0.2	0.1
2	3	3	9	1,932.9	1,774.8	1,774.8	8.9	0	0.2	0.1
3	3	3	9	1,246.6	1,123.3	1,123.3	11	0	0.2	0
4	10	4	40	2,541.0	2,440.8	2,440.8	4.1	0	0.2	0.1
5	10	4	40	51,221	51,031	51,031	0.4	0	2	0.3
6	10	4	40	51,838	51,450	51,443	0.8	0	2	0.3
7	38	4	152	648.6	529.8	486.2	22.4	8.2	1,205	1.4
Average		4					6.9	1	151.5	0.3
8	3	6	18	2,349.8	2,196.5	2,196.5	7	0	0.5	0.1
9	3	6	18	2,325.8	2,133.5	2,133.4	9	0	0.5	0.1
10	3	6	18	1,541.3	1,387.9	1,387.9	11	0	0.5	0.1
11	10	6	60	3,151.6	3,019.1	3,019.1	4.4	0	0.5	0.1
12	10	6	60	67,577	67,323	67,322	0.4	0	5.2	0.5
13	10	6	60	68,211	67,746	67,660	0.7	0.1	6.7	0.5
14	10	6	60	68,715	68,428	68,420	0.4	0	5	0.5
15	38	6	228	1,078.5	937.4	919.1	15.1	2	> 3,214	2.9
Average		6					6	0.3	> 404	0.6
16	3	8	24	2,616.4	2,451.4	2,451.1	6.7	0	0.8	0.2
17	3	8	24	2,605.5	2,403.2	2,402.8	8.4	0	0.9	0.1
18	3	8	24	1,748.6	1,583.9	1,583.3	10.4	0	0.8	0.2
19	10	8	80	3,541.2	3,395.7	3,395	4.3	0	0.8	0.1
20	10	8	80	72,277	71,920	71,896	0.5	0	24.3	0.7
21	10	8	80	72,957	72,370	72,327	0.8	0.1	50.2	0.9
22	10	8	80	72,191	71,854	71,810	0.5	0.1	13	0.9
23	38	8	304	1,503.3	1,356.9	1,348.8	10.8	0.6	> 4,767	5.2
Average		8					5.3	0.1	> 607	1
Grand average							6.1	0.5	> 387	0.7

**Table 2. Size Characteristics of Generated Problems**

Problem ( <i>n-N-C</i> )	MILP Model Size		
	Binary Variables	Continuous Variables	Total Constraints
10-10-15	100	511-551	451
10-10-20	100	591-631	501
10-15-15	150	671-711	601
10-15-20	150	771-811	651
15-10-15	150	781-676	676
15-10-20	150	841-946	751
15-15-15	225	1,051-1,066	901
15-15-20	225	1,186-1,201	976
20-10-15	200	1,061-1,101	901
20-10-20	200	1,161-1,241	1,001
20-15-15	300	1,361-1,421	1,201
20-15-20	300	1,541-1,621	1,301

state-of-the-art integer optimizer CPLEX [the exact solutions are taken from Liu and Sahinidis (1996) who used a specialized solution algorithm]. Clearly, the heuristic produces excellent-quality solutions while being very fast.

In Tables 2 and 3, we refer to 12 different sets of test problems generated using the test problem generator described in Liu et al. (1996). The first column of Table 2 gives the size of the corresponding chemical process networks in the form *n-N-C*. In the same table, we give the number of binary and continuous variables, and the number of rows in the constraint matrix. Each set comprises eight randomly generated problems. Whereas the number of binaries and constraints is fixed according to *n-N-C* for each problem set, we present the number of continuous variables in the constraint matrix using ranges, since these quantities vary according to the network structure of each randomly generated problem, that is, according to the number of interconnections between processes.

Table 3 provides the CPU requirements for the 12 generated problem sets for the exact and heuristic algorithm as well as the percentage difference between the exact and heuristic values  $[(z - z^H/z) \times 100]$ . We present the minimum,

maximum, and average over all eight generated problems for each problem size. The heuristic approximation error is only 0.5%, on the average, whereas the running time of the heuristic is several orders of magnitude less than the time required for solving the integer program.

The theoretical results of the previous sections predicted that, as the number of time periods of the problem increases, the linear-programming relaxation gap decreases and the heuristic comes closer to being optimal. This is indeed demonstrated by both Tables 1 and 3, which show that asymptotic analytical results provide useful information even for realistic problem sizes.

## Conclusions

The main purpose of this article has been to introduce and motivate the further development of analytical investigations of heuristic and exact algorithms in process synthesis and process operations. The approach has been demonstrated for the multiperiod design and expansion of chemical process networks. Under certain assumptions about the problem inputs, the linear-programming relaxation gap of an integer model for this problem was shown to vanish as the size of the problem grows. This analysis motivated the development of a heuristic that was proven to be asymptotically optimal. An extensive computational study verified the theoretical predictions.

The results in this article can be extended in a number of different directions in the context of process capacity expansion, time-discretized formulations of process planning and scheduling problems, and other process synthesis and operations problems.

In the context of the capacity expansion problem, one can embed the proposed heuristic within a Lagrangian relaxation scheme to obtain solutions for problems with additional constraints, such as investment constraints, omitted here for simplicity. One can also improve the heuristic rounding scheme by optimally allocating capacity over time independently for each process after the network mass flows are fixed according to the relaxed problem solution. Perhaps more important

**Table 3. Computational Results for Generated Problems**

Problem ( <i>n-N-C</i> )	CPU s for IP			CPU s for Heuristic			$(z - z^H/z) \times 100$		
	Min.	Avg.	Max.	Min.	Avg.	Max.	Min.	Avg.	Max.
10-10-15	2	9	24	1	1	2	0	1.1	3
10-10-20	3	52	236	1	2	3	0	0.4	1.4
10-15-15	8	31	65	2	3	4	0	0.8	3.2
10-15-20	2	76	244	2	4	7	0	0.5	0.9
Average	4	42	142	1.5	2.5	4	0	0.7	2.1
15-10-15	8	127	721	2	4	5	0	0.5	1.5
15-10-20	23	63	133	4	4	6	0	0.3	0.6
15-15-15	39	627	2,403	6	8	10	0.1	0.6	1.1
15-15-20	113	533	1,254	10	11	15	0	0.4	1
Average	46	337	1,128	5.5	7	9	0	0.5	1
20-10-15	12	102	417	4	6	8	0	0.3	0.7
20-10-20	10	50	93	5	7	8	0	0.2	0.8
20-15-15	54	1,978	8,293	10	17	23	0.1	0.4	1.3
20-15-20	83	1,373	3,794	14	25	38	0.2	0.4	0.9
Average	40	878	3,150	8	11	20	0.1	0.3	0.9
Grand average		418			8			0.5	

would be the development of asymptotic probabilistic results for the case when the number of processes of the network increases.

For time-discretized models of process planning and scheduling problems, one should address the question whether finer discretizations of *multiperiod* formulations improve the quality of linear programming relaxation bounds. Similar questions should be addressed in the context of *multistage* formulations of synthesis problems.

Analytical investigations for other process synthesis and operations problems appear particularly promising. These investigations should begin with a formal computational complexity analysis of these problems. Such an analysis is useful for two reasons. First, the mere fact that the number of alternatives in, for example, distillation (heat exchanger) network synthesis increases exponentially as the number of products (streams) involved is increased, does not necessarily imply that distillation (heat exchanger) network synthesis cannot be solved in polynomial time. Certain polynomially solvable problems also exhibit an exponential increase in candidate solutions as the size of the problem increases (for example, the number of extreme points of a linear program increases exponentially with the number of variables and constraints). Second, complexity proofs are based on reduction between problems, thus providing useful relationships between different design and optimization problems when reductions preserve approximability.

Our conjecture is that most process synthesis and operations problems cannot be solved in polynomial time. Therefore, the development of probabilistic and worst-case analysis results for these problems can be expected to lead to significant new insights to algorithmic, heuristic, and problem structure, and motivate the design of new heuristics with provably good performance.

This article has shown that theoretical analysis of the linear programming relaxation of optimization formulations can play a key role in all the directions just mentioned.

## Acknowledgments

The work of the first author (M. L. L.) was partially supported by the National Science Council, Taiwan, under award NSC 86-2115-M-004-002. The second author (N. V. S.) was partially supported by the National Science Foundation under CAREER Award DMI 95-02722.

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## Appendix

**Theorem 1.** For any realization of coefficients of  $P_n$ , we have

$$z_n^L - N \times n \times \beta_{\max} \leq z_n \leq z_n^L$$

where  $\beta_{\max} = \max_{i,j} \{\beta_{ij}\}$ .

**Proof.** Let  $\{X^*, Q^*, W^*, P^*, S^*, y^*\}$  be optimal to  $P_n^L$ . Then,  $\{X^*, Q^*, W^*, P^*, S^*, [y^*]\}$  is a feasible solution of  $P_n$  obtained by fixing the fractional components of  $y^*$  at 1. Therefore



$$\begin{aligned}
z_n^L - z_n &\leq - \sum_{i=1}^N \sum_{t=1}^n \beta_{it} y_{it}^* + \sum_{i=1}^N \sum_{t=1}^n \beta_{it} [y_{it}^*] \\
&= \sum_{i=1}^N \sum_{t=1}^n \beta_{it} ([y_{it}^*] - y_{it}^*) \\
&\leq \sum_{i=1}^N \sum_{t=1}^n \beta_{it} \\
&\leq N \times n \times \beta_{\max}.
\end{aligned}$$

**Theorem 2.** Let  $K$  be the number of fractional components of  $y$  in an optimal solution of  $P_n^L$ . Then, there exists an optimal solution of  $P_{n+1}^L$  with  $K$  fractional components in  $y$  w.p. 1.

*Proof.* For notational simplicity, we omit the indices of  $i$ ,  $j$ , and  $l$  whenever possible. Let  $Z_n^* = \{X^*, Q^*, W^*, P^*, S^*, y^*\}$  be an optimal solution of  $P_n^L$  with  $K$  fractional components in  $y^*$ . We will use  $Z_n^*$  to construct a feasible solution to  $P_{n+1}^L$  with the same number of fractional components, and subsequently prove that the constructed solution is optimal.

Without loss of generality, let us partition the last time period of  $P_n$  to construct  $P_{n+1}$ . Let  $Z'_{n+1} = \{X', Q', W', P', S', y'\}$  be a vector in  $P_{n+1}^L$  space. Construct  $Z'_{n+1}$  in the following way:

$$\left\{ \begin{array}{l} X'_t = X_t^*, Q'_t = Q_t^*, W'_t = W_t^* \\ P'_t = P_t^*, S'_t = S_t^*, y'_t = y_t^* \end{array} \right\} \quad t = 1, \dots, n-1; \quad \forall i, j, l \quad (A1)$$

$$\left\{ \begin{array}{l} X'_n = X_n^*, Q'_n = Q_n^*, W'_n = \frac{1}{2} W_n^* \\ P'_n = \frac{1}{2} P_n^*, S'_n = \frac{1}{2} S_n^*, y'_n = y_n^* \end{array} \right\} \quad \forall i, j, l \quad (A2)$$

and

$$\left\{ \begin{array}{l} X'_{n+1} = 0, Q'_{n+1} = Q_n^*, W'_{n+1} = \frac{1}{2} W_n^* \\ P'_{n+1} = \frac{1}{2} P_n^*, S'_{n+1} = \frac{1}{2} S_n^*, y'_{n+1} = 0 \end{array} \right\} \quad \forall i, j, l. \quad (A3)$$

It is clear that  $Z'_{n+1}$  has  $K$  fractional components in  $y'$  and is feasible to  $P_{n+1}^L$ . Let  $V_n^*$  be the objective function value of  $Z_n^*$  and  $V'_{n+1}$  be the objective function value of  $Z'_{n+1}$ . Then, by taking the expectation of the objective function:

$$\begin{aligned}
E(V'_{n+1}) &= E \left[ \sum_{t=1}^{n+1} (\gamma_t S'_t - \Gamma_t P'_t) \right] \\
&\quad - E \left[ \sum_{t=1}^{n+1} (\alpha_t X'_t + \beta_t y'_t + \delta_t W'_t) \right] \\
&= E(V_n^*).
\end{aligned}$$

We now claim that no other feasible solution to  $P_{n+1}^L$  and therefore no solution with more than  $K$  fractional components has a better objective function than that of  $Z'_{n+1}$ . Indeed, consider any  $\hat{Z}_{n+1}$  that is feasible to  $P_{n+1}^L$ . Let  $\hat{V}_{n+1}$  be the objective function value of this solution. From Eqs. A1, A2, and A3 we know that summing the  $n$ th and  $(n+1)$ th time period values into the  $n$ th time period of  $\hat{Z}_{n+1}$  and projecting onto  $P_n$  space yields a feasible solution to  $P_n^L$ . Let us construct such a solution  $Z''_n$ . We consider two cases:

1. If  $\hat{y}_n + \hat{y}_{n+1} > 1$ , set  $y''_n$  to 1, then

$$\begin{aligned}
E(\hat{V}_{n+1}) &= E \left[ \sum_{t=1}^{n+1} (\gamma_t \hat{S}_t - \Gamma_t \hat{P}_t) - \sum_{t=1}^{n+1} (\alpha_t \hat{X}_t + \beta_t \hat{y}_t + \delta_t \hat{W}_t) \right] \\
&= E \left[ \sum_{t=1}^n (\gamma_t S''_t - \Gamma_t P''_t) - \sum_{t=1}^n (\alpha_t X''_t + \beta_t y''_t + \delta_t W''_t) \right] \\
&\quad - E(\beta_{n+1} \hat{y}_{n+1} + \beta_n \hat{y}_n - \beta_n y''_n) \\
&< E(V_n^*) \\
&= E(V'_{n+1}).
\end{aligned}$$

2. If  $\hat{y}_n + \hat{y}_{n+1} \leq 1$ , set  $y''_n = \hat{y}_n + \hat{y}_{n+1}$ , then

$$\begin{aligned}
E(\hat{V}_{n+1}) &= E \left[ \sum_{t=1}^{n+1} (\gamma_t \hat{S}_t - \Gamma_t \hat{P}_t) - \sum_{t=1}^{n+1} (\alpha_t \hat{X}_t + \beta_t \hat{y}_t + \delta_t \hat{W}_t) \right] \\
&= E \left[ \sum_{t=1}^n (\gamma_t S''_t - \Gamma_t P''_t) - \sum_{t=1}^n (\alpha_t X''_t + \beta_t y''_t + \delta_t W''_t) \right] \\
&\leq E(V_n^*) \\
&= E(V'_{n+1}).
\end{aligned}$$

In both cases, we have  $E(\hat{V}_{n+1}) \leq E(V'_{n+1})$ . Therefore, the constructed solution with  $K$  fractional components in  $y$  is optimal to  $P_{n+1}^L$ .

**Theorem 3.** Let  $K$  be the number of fractional components of  $y$  in an optimal solution of  $P_{n_0}^L$  for any number of time periods  $n_0$ . Then,

$$z_n^L - z_n \leq K \times \beta^U \quad \text{w.p. 1,} \quad \forall n > n_0.$$

*Proof.* From Theorems 1 and 2 we have

$$z_n^L - K \times \beta_{\max} \leq z_n \leq z_n^L \quad \forall n > n_0. \quad (A4)$$

Since  $\beta_t \leq \beta^U$ , we have  $E(\beta_t) \leq \beta^U, \forall t$ . Hence,  $E(\beta_{\max}) \leq \beta^U$ . From this observation and Eq. A4 the theorem follows easily.

**Theorem 4.** There exists a number  $n_0$  such that  $\forall n > n_0$ , the solution of  $P_n^L$  has no more fractional components than the number of fractional components in the solution of  $P_{n_0}^L$  w.p. 1.

**Proof.** For those realizations of supplies and demands for which the mass balances, Eqs. 5–8, are infeasible, the solution of  $P_n$  involves no expansions and the theorem is satisfied trivially. For any feasible realization of  $a_{jlt}^L$ ,  $a_{jlt}^U$ ,  $d_{jlt}^L$ , and  $d_{jlt}^U$ , consider the following problem:

$$\omega_{it} = \max W_{it},$$

subject to

$$\sum_{l=1}^M P_{jlt} + \sum_{i'=1}^N \eta_{ij} W_{i't} = \sum_{l=1}^M S_{jlt} + \sum_{i'=1}^N \mu_{ij} W_{i't} \quad j = 1, \dots, C$$

$$a_{jlt}^L \leq P_{jlt} \leq a_{jlt}^U \quad j = 1, \dots, C; \quad l = 1, \dots, M$$

$$d_{jlt}^L \leq S_{jlt} \leq d_{jlt}^U \quad j = 1, \dots, C; \quad l = 1, \dots, M$$

$$W_{i't} \geq 0 \quad i' = 1, \dots, N$$

$$P_{jlt} \geq 0 \quad j = 1, \dots, C; \quad l = 1, \dots, M$$

$$S_{jlt} \geq 0 \quad j = 1, \dots, C; \quad l = 1, \dots, M.$$

Since the random variables of demand and availability are bounded,  $E(\omega_{it})$  are finite numbers for all  $i$  and  $t$ . Let  $U_i$  denote the maximum possible values for  $E(\omega_{it})$ .

Suppose that we start by drawing a problem  $P_{n_1}$  with  $n_1$  time periods. After solving  $P_{n_1}^L$ , we now consider the total installed capacity of the last time period,  $Q_{in_1}$ ,  $i = 1, \dots, N$ . If the constraints

$$U_i \leq \tau_{n_1} Q_{in_1} \quad i = 1, \dots, N \quad (\text{A5})$$

are satisfied, then there is no need for additional expansion for the larger size problems. Setting  $n_0 = n_1$  proves the theorem. If one of the constraints (Eq. A5) is not satisfied, then we expand the problem. Due to constraints (Eqs. 2 and 3),  $Q_{it}$  does not decrease as  $t$  increases. In particular, for sufficiently large problem size, the parameters for supplies and demands corresponding to the expected maximum possible capacity requirements will be eventually drawn. Therefore, by repeating the growing procedure many times, there exists a number  $n_0$  such that constraints (Eq. A5) are satisfied in expectation. Therefore, additional time periods will not lead to any additional capacity expansions and hence any additional fractional  $y$  values.

**Theorem 5**

$$\lim_{n \rightarrow \infty} \left( \frac{z_n^L}{n} - \frac{z_n}{n} \right) = 0 \quad \text{w.p. 1.}$$

**Proof.** Let  $K$  be the number of fractional components of  $y$  in a solution of  $P_{n_0}^L$ . From Theorem 4, Eq. A4 is also satisfied for the infinite horizon case. Division of Eq. A4 by  $n$  yields

$$\frac{z_n^L - K \times \beta_{\max}}{n} \leq \frac{z_n}{n} \leq \frac{z_n^L}{n}. \quad (\text{A6})$$

Since  $\beta_t \leq \beta^U$ , we have  $E(\beta_t) \leq \beta^U$ ,  $\forall t$ . Hence,  $E(\beta_{\max}) \leq \beta^U$ . From this observation and Eq. A6, asymptotic equivalence of  $z_n/n$  and  $z_n^L/n$  w.p. 1 follows easily.

**Theorem 6.** The solution  $\bar{x}$  obtained by the preceding heuristic is feasible to  $P$  and  $z^H \leq z \leq z^L$ .

**Proof.** We will show that the solution  $\bar{x}$  obtained from the heuristic satisfies all constraints (Eqs. 2–9). Since  $x^*$  solves the relaxation,  $x^*$  satisfies all constraints except for constraint (Eq. 9). In the beginning of the heuristic, we set  $x^*$  to  $\bar{x}$ , and throughout the heuristic the components  $\bar{W}$ ,  $\bar{P}$ , and  $\bar{S}$  of  $\bar{x}$  are not changed. Hence, constraints (Eqs. 5–7) are still satisfied by  $\bar{x}$ . From Steps 3.1 and 3.2, the heuristic forces  $\bar{y}_{it}$  to either 1 or 0, which guarantees that Eq. 9 will be satisfied. Step 3.2, forces the values of  $\bar{X}_{it}$  not to exceed  $X_{it}^U$  when  $\bar{y}_{it} = 1$ , whereas  $\bar{X}_{it} = 0$  when  $\bar{y}_{it} = 0$ . Hence, constraint (Eq. 2) will also be satisfied. From Step 5, Eq. 3 is satisfied. Finally, we need to check whether  $Q_{it}^* \leq \bar{Q}_{it}$ ,  $\forall i, t$ . Indeed, from constraint Eq. 3, we have  $Q_{it} = \sum_{i'=1}^I X_{i't}$ . Then,

$$Q_{it}^* = \sum_{i=1}^I X_{it}^* \leq \sum_{i=1}^I \bar{X}_{it} = \bar{Q}_{it}.$$

This inequality shows that constraint (Eq. 4) will be satisfied. Therefore,  $\bar{x}$  is feasible for  $P$  and  $z^H \leq z \leq z^L$ .

**Theorem 7**

$$E(z_n^L - z_n^H) \leq N \times \beta.$$

**Proof.** Taking the expectation of both sides of Eq. 11 yields

$$\begin{aligned} E(z_n^L - z_n^H) &= E \left[ \sum_{i=1}^N \sum_{t \in T_i} (\alpha_{it} \bar{X}_{it} + \beta_{it} \bar{y}_{it}) \right] \\ &\quad - E \left[ \sum_{i=1}^N \sum_{t \in T_i} (\alpha_{it} X_{it}^* + \beta_{it} y_{it}^*) \right] \\ &= \alpha \sum_{i=1}^N \sum_{t \in T_i} (\bar{X}_{it} - X_{it}^*) \\ &\quad + \beta \sum_{i=1}^N \sum_{t \in T_i} (\bar{y}_{it} - y_{it}^*) \end{aligned}$$

From the heuristic, it is easy to verify that

$$\sum_{t \in T_i} (\bar{X}_{it} - X_{it}^*) = 0 \quad i \in \{1, \dots, N\}$$

and

$$\sum_{t \in T_i} (\bar{y}_{it} - y_{it}^*) \leq 1 \quad i \in \{1, \dots, N\}. \quad (\text{A7})$$

Therefore, the theorem follows.

The last step of the proof of the preceding theorem clearly

shows that Eq. A7 is *not* satisfied if one simply rounds up all the  $y_{it}$  variables that are fractional in the relaxed problem solution.

*Theorem 8*

$$\lim_{n \rightarrow \infty} (z_n^L - z_n^H) \leq N \times \beta \quad \text{w.p. 1.}$$

*Proof.* Let  $\bar{x}_{n_0}$  be the solution obtained by heuristic for problem  $P_{n_0}$ . From Theorem 7, we have

$$E(z_n^L - z_n^H) \leq N \times \beta \quad \forall n > n_0.$$

Then, the theorem follows easily.

*Theorem 9*

$$\lim_{n \rightarrow \infty} \left( \frac{z_n^L}{n} - \frac{z_n^H}{n} \right) = 0 \quad \text{w.p. 1.}$$

*Proof.* Similar to Theorem 7.

*Manuscript received Nov. 7, 1996, and revision received May 5, 1997.*

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