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Comparing structural constraints for accelerated branch and bound solver of process network synthesis problems*

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Abstract

The P-graph methodology can be used to find the optimal solution for large process systems. This methodology solves the combinatorial part of the problem more efficiently than the traditional branch and bound method due to the relationships inherent in the structure. However, reducing the number of possibilities developed in the constraint functions also plays a major role in this algorithm. In this publication, we present a new constraint function that also takes into account the minimum cost structure and compares it with earlier versions.

Introducion

The task of process network synthesis is to determine the optimal structure of a process system, the optimal configurations, and operating sizes of the functional units that make up the system and perform various operations [2]. Process synthesis plays a critical role in reducing material, energy consumption, and negative environmental impacts, thereby increasing profitability.

Ideally, the structure of a process and the operational configurations that make up the process could be designed and synthesized simultaneously because their

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performance interacts. In practice, however, it is extremely difficult due to the simultaneous continuous and discrete nature of the task. The discrete nature is caused by the structure of the process, which leads to the combinatorial complexity of the problem that makes it complex to find an optimal solution to the problem. The process network synthesis problems formulate a MILP problem with many binary variables. Finding the optimal subnetwork is an NP-hard problem.

Combinatorial analysis can be applied to this type of problems. The method is used to reduce the number of possible solutions by exploiting the unique properties of the so-called PNS (Process Network Synthesis) problems is the ABB (Accelerated Branch and Bound) method [1]. It is based on the branch and bound method, i.e., the method uses a lower bound submethod to exclude solutions that cannot provide a better solution than the currently known best solution. It is critical for the computation time of solving the problem with the B&B method to find a tighter lower bounding submethod. The currently available implementations and the previous studies do not exploit all the information, considering only the continuous part of the problem by calculating the LP relaxation of the MILP problem. In this article, we introduce a better lower bounding sub-method taking into consideration not just the continuous but also the structural nature of the PNS problem.

Mathematical model for P-Graph

The continuous variables of the model are denoted by x and the binary variables by y. These variables are assigned to operational units. The continuous variable x_i indicates the operational size of the operational unit $O_i(\in O)$, and the binary variable y_i indicates whether the unit is in the structure or not.

The objective function is to minimize cost. The cost is composed of the investment cost, the operating cost of the operational units, and the price of the raw material. These components cover the full cost of the network, i.e., the process to be synthesized considers the full cost.

In addition to the capacity constrains listed above, additional constraints are imposed on material balances, products, and raw materials. For products, we usually set lower limits to determine how much we need to produce at least of a given product, while for raw materials we may set upper limits if these types of raw material quantities are not available in unlimited amount. Material balance conditions should be defined for intermediate products.

Illustration of new constrain

The following simple example illustrates the efficiency of our algorithm. In our example, we want to produce one product (D) from the raw material (A), using the operating units $O_1, O_2, \ldots, O_5$.

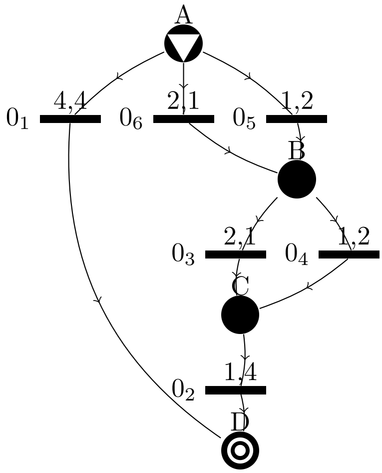

Figure 1. A simple p-graph in which the fixed and proportional costs are visible above the operating units.

The final product (D) can be produced by either O_1 or O_2 or both operating units. If the machine 0_1 chooses to produce the D final product. In this case the O_1 unit consumes only the A raw material. The total production cost will be the sum of the fixed and proportional costs of the O_1 operating unit. The optimal solution is $y_1 = 1, x_1 = 1$ and the other variables are 0.

Consider another branch that chooses O_2. In this case, our previous production cost is $1+4$, because $y_2 = 1$ and $x_2 = 1$. In the original version, the operating cost of producing C is added to this cost. The optimal solution for $x_3 = 1$ and $x_6 = 1$ is 2. For the lower bound, we obtain a value of 7, which is smaller than the previous value of 8. That is, this branch is explained by the previous constraints. However, structurally, the minimum cost of the operating units needed to produce C is 2, which is the minimum in the $y_4 = 1$ and $y_5 = 1$ case. Then the installation cost of $1 + 1$ is added to $5 + 2$. So, in total, the lower bound is 9, which is already worse than 8. With this new lower bound, ABB algorithm is not explained this case.

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