Strengthening Mathematical Formulation for Global Optimization of the Operational Water Network Distribution

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Pump scheduling is a decision-making problem in water distribution networks. The aim is to plan the pumping operations to minimize the energy cost over the day ahead. Modelling the binary status of the pumps and the nonconvex head-flow relations throughout the network results in nonconvex Mixed Integer Nonlinear programs (MINLP) that could be particularly hard to solve. The branch-and-check algorithm implemented on top of a commercial linear solver to guarantee the global optimization paradigm is viable due to convexification of malign constraints. The looseness of convexifications exacerbates the convergence of the optimization process. In response to these caveats, we propose a tailored bound tightening and generation of valid inequalities at the preprocessing stage. The promising computational results over a set of benchmarks indicate the effectiveness of our approach.

Mots-clés : *integer nonconvex programming, bound tightening, cutting plane, pump scheduling*

1 Introduction

This paper draws attention to strengthening mathematical formulations for global optimization of the pump scheduling problem in drinking water distribution networks via bound tightening and cut generation. The pump scheduling problem deals with satisfying a forecasted demand for a determined time horizon, e.g., the day after, via discretized decision making (planning status on/off of the pumps) for each time step within the horizon. Besides integrality, the mathematical formulations suffer from the hydraulic nonlinear relationship between flow and head (pressure) in pipes and pumps. Despite recent advances in global optimization solvers, simultaneous handling of both nonlinearity and integrality remains intractable for relatively large-scale problems. To realize the global optimization of the problem, [2, 9] present a branch-and-check framework : Given a polyhedral outer approximation (OA) of the nonconvex head-flow constraints, the resulting MILP relaxation is solved with a standard branch-and-bound. At each integer node of the search tree, the feasibility and the real cost of the relaxed integer solution is checked. In case of infeasibility a no-good combinatorial cut is generated. In this framework, a stronger MILP relaxation surely leads to check less infeasible solutions and to a quicker convergence of the optimization process. As the OA relaxations directly rely on the variable bounds, bound tightening may not only help to reduce the search domain but it allows to reshape the MILP relaxation.

In this short paper, we first present applications of the optimization-based bound-tightening (OBBT) [3] principle. We discuss how to define both efficient and effective auxiliary optimization problems by selecting suited relaxations, restrictions, and conditions. Second, we propose to address the combinatorial complexity of the pump scheduling problem, also by studying the substructures of the network, to identify valid inequalities to improve the LP relaxation. Our experiments on two networks of the literature show the deep impact of this enhanced preprocessing on the results of the exact method from [2].

2 Mathematical formulation

We briefly present a mathematical model for the pump scheduling problem. More details can be found, e.g., in [2, 9]. A water distribution network can be formalized as a directed graph $G = (J, A)$: arcs $a \in A$ are either pipes $a \in A_L$ or pumps $a \in A_K$, and nodes $j \in J$ represent either sources $j \in J_S$, or service nodes (also called junctions) $j \in J_J$, or water tanks $j \in J_R$. The scheduling horizon is discretized in typically $T = 24$ hourly time steps : $t \in \mathbb{T}$, with $\mathbb{T} = \{0, \ldots, T-1\}$. Some arcs are controllable, namely fixed-speed pumps and pipes equipped with gate valves, and have two possible states (i.e., on or off) at each time instant t. This is formulated as a boolean variable : $x_{at} = 0$ if arc $a \in A$ is inactive (i.e., flow cannot pass) and $x_{at} = 1$, otherwise. Each arc $a \in A$ between the nodes i and j is also associated with a function ϕ_a, which relates the flow $q_{at} \in \mathbb{R}$ with the head (potential) loss $v_{at} = h_{it} - h_{jt} \in \mathbb{R}$ at time $t \in \mathbb{T}$. The head h_{jt} at a water tank j is proportional to the filling level, which is limited by the tank capacity. The pump scheduling problem can be stated as :

$$(P) : min \quad \sum_{\mathbb{T}} \sum_{A_K} c^0_{at} x_{at} + c^1_{at} q_{at} \tag{1}$$

$$s.t. : \quad q_{jt} = D_{jt} \qquad \forall j \in J_L, t \in \mathbb{T} \tag{2}$$

$$h_{jt+1} = h_{jt} + \sigma_j q_{jt}, \qquad \forall j \in J_T, t \in \mathbb{T} \tag{3}$$

$$\underline{Q}_{at} x_{at} \leq q_{at} \leq \overline{Q}_{at} x_{at} \qquad \forall a \in A, t \in \mathbb{T} \tag{4}$$

$$\phi_a(q_{at}) + \underline{V}_{at}(1 - x_{at}) \leq v_{at} \leq \phi_a(q_{at}) + \overline{V}_{at}(1 - x_{at}) \qquad \forall a \in A, t \in \mathbb{T} \tag{5}$$

$$\underline{H}_{jt} \leq h_{jt} \leq \overline{H}_{jt} \qquad \forall j \in J_T, t \in \mathbb{T} \tag{6}$$

$$x \in X \in \{0,1\}^{A \times \mathbb{T}}. \tag{7}$$

The objective function is to minimize the electricity cost of pumping and the constraints describe, at each time step : (2) demand satisfaction at junctions j where $q_{jt} = \sum_{a \in A} q_{at}$ is the residual flow, (3) flow conservation at tanks, (4) flow bounds w.r.t. arc status, (5) potential-flow relation w.r.t arc status, (6) tank capacities, (7) any additional linear condition on the controllable arcs (e.g., dependencies between parallel pumps or usage limits). Disjunctions on the arc activity are modeled in constraints (4)-(5) using 'big-M' values : $\underline{Q} \leq \overline{Q}$ denote bounds on the flows q in active arcs, and $\underline{V} \leq \overline{V}$ denote bounds on the head loss v in inactive arcs. The exact method [2] for solving (P) is based on a MILP relaxation, obtained by replacing in (5), the nonlinear term $\phi_a(q_{at})$ with polyhedral under- and over-estimators $\underline{\phi}_a(q_{at})$ and $\overline{\phi}_a(q_{at})$ as illustrated in Figure 1. We denote with R the LP-relaxation feasible set.

3 Optimization-Based Bound tightening

In this section, we present feasibility-oriented and optimization-based bound tightening techniques for preprocessing the LP relaxation $\mathcal{R}$, i.e., we rely on minimizing/maximizing a variable on a suited relaxation of (P) to derive the lower/upper bounds of the variable. For any such auxiliary problem, we denote with $\mathcal{O}$ its relaxed feasible set, as opposed to the relaxed set $\mathcal{R}$. The choice of relaxation $\mathcal{O}$ is very sensitive : too tight and solving one auxiliary problem may be as hard as solving (P), too loose and it provides no new information to $\mathcal{R}$ that the optimization process cannot infer alone. Still, as the OBBT procedure runs all the auxiliary problems in a row, a bound reduction, even if obtained with a loose relaxation, will be propagated to the next auxiliary problems.

3.1 Single-period relaxation for control variables

The only temporal coupling constraint is (3). Relaxing these constraints will decompose each time step. Therefore, each time interval $t \in \mathbb{T}$ can go under scrutiny independently while the levels of the tanks at time step t and $t+1$ are within their box constraints $[\underline{H}_{jt}, \overline{H}_{jt}]$ and still respect constraint $[\underline{Q}_{at}, \overline{Q}_{at}]$ merely for this time interval. We consider this single-period relaxation $\mathcal{O}_t$ to compute the bounds on the stationary flow q_{at} and head loss v_{at} variables. It is still discrete and nonconvex but of very small size. Furthermore, we enforce condition $x_{at} = 1$ in $\mathcal{O}_t$ to compute the flow bounds

$\underline{Q}_{at}, \overline{Q}_{at}$ of constraints (4). If the auxiliary problem is infeasible then x_{at} can be turned into constant 0 in the MILP relaxation. Similarly, the head-loss bounds $\underline{V}_{at}, \overline{V}_{at}$ of constraints (5) are computed by enforcing $x_{at} = 0$ in $\mathcal{O}_t$, and, if infeasible, x_{at} is fixed to 1 in the model. This principle, known as probing [8], allows reducing both the big-M values and the number of binary variables in $\mathcal{R}$.

3.2 Multi-period relaxation for state variables

One major feasibility issue in (P) comes from the tank capacities in constraints (6). Thus, tight bounds $\underline{H}, \overline{H}$ on the water level in the tanks impact the strength of both $\mathcal{R}$ and the single-step relaxations $\mathcal{O}_t$ used in our iterative OBBT procedure (Sec. 3.1). We also evaluate the bounds on the difference of level between two tanks as it fully determines the flow passing between them (if there is no intermediate tank in the paths). The concluded bounds would be added as a new class of constraints in the subsequent auxiliary problems of the OBBT procedure.

The single-step relaxation is not relevant to evaluate these bounds since the water level at time t depends on the decisions made at the other periods. We thus consider a multi-period relaxation $\mathcal{O}$ instead. The period length (from 2 to T) and the strength of $\mathcal{O}$ (with or without nonconvex or integrality constraints) are chosen according to the size of the network.

4 Valid inequalities

4.1 Disjunctions and related network elements

In water networks, a tank $j \in J_T$ is often fed through a controllable arc $a \in A$ (e.g. a pump or/and a valve). We propose then to use probing to compute conditional bounds on the level of the tank and strengthen constraints (6) with

$$h_{jt} \geq \underline{H}^1_{jt} x_{at} + \underline{H}^0_{jt}(1 - x_{at}).$$

We apply this principle also to relate the flow through a pipe $a \in A$ with the status of controllable arcs in a same branch. Probing on these status allows sometimes to significantly reduce the bounds on q_{at} and even result in disjunctive regions. The OA of constraints (5) can then be greatly improved using these conditional bounds as depicted in Figure 1. Moreover, such conditional bounds can usually be inferred for free from bounds computed in the OBBT procedure and flow conservation in the considered branch.

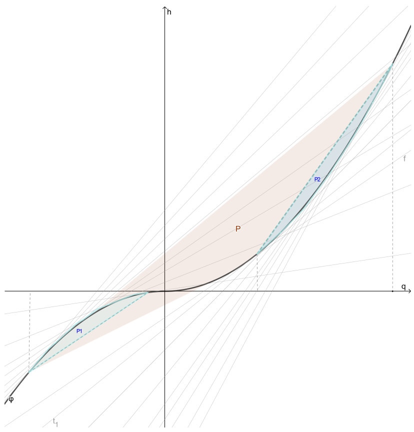

FIG. 1 – OA for constraint (5) in orange and its refinement in blue from probing

4.2 Cardinality cuts

OBBT applies not only to decision variables y but also to any (linear) variable composition $f(y)$. The resulting bounds are then enforced in (P) with additional linear constraints, e.g., $f(y) \geq \underline{F}$. Again, this procedure must be reserved for some promising compositions. We applied it to the minimum total of active pumps $\sum_{a\in A,t\in\bar{\mathbb{T}}} x_{at}$ with $\bar{\mathbb{T}} \subset \mathbb{T}$. The intuition behind this choice is : (i) pushing up this lower bound mechanically increases the objective cost on $\mathcal{R}$, (ii) limiting the period length in $\mathcal{O}$ (to $[0,\tau]$ or $[\tau, T]$) ensures its tractability, (iii) less flexibility is given to $\mathcal{O}$ when restricted to those intervals as the level of the tanks is fixed at times 0 and T, (iv) since the number of active pumps (corresponding to $f(y)$ here) is an integer, we can apply a Mixed-Integer Rounding (MIR) technique [13] to lift the constraint above as follows :

$$f(y) \geq \frac{1}{\underline{F} - \lfloor \underline{F} \rfloor} * S(y - y^*) + \lceil \underline{F} \rceil,$$

where y^* denotes an optimal solution of the OBBT problem $\min_{y\in\mathcal{O}} f(y)$, $\underline{F} = f(y^*)$ is the optimum value, and S is a gradient of f at y^*. If relaxation $\mathcal{O}$ is an LP, then gradient S is directly derived from an optimal dual solution.

4.3 Flow cutset-based inequalities

By collapsing some demand nodes and at least one tank node $j \in J_T$, we derive a supernode $v \subset J$, the aggregate demand $d_{vt} = \sum_{j'\in v} d_{j't}$, and the sets of ingoing arcs A_v^- and outgoing arcs A_v^+ (e.g, see figure 2). We then introduce a cutset-based inequality [4] at which the flow is projected out by utilizing the capacities of each arc. Hence, combining constraints (2-4) over periods $t \in \mathbb{T}' = \{t', t'+1, ..., t'+\tau\} \subseteq \mathbb{T}$, we get :

$$\sum_{a\in A_v^-} \sum_{t\in\mathbb{T}'} \overline{Q}_{at} x_{at} - \sum_{ij\in A_v^+} \sum_{t\in\mathbb{T}'} \underline{Q}_{at} x_{at} + \frac{1}{\sigma_j}(h_{jt'} - \underline{H}_{j(t'+\tau+1)}) \geq \sum_{t\in\mathbb{T}'} d_{vt}. \tag{8}$$

To strengthen these cutset-based inequalities, initially, we select a subset of arcs to construct cover

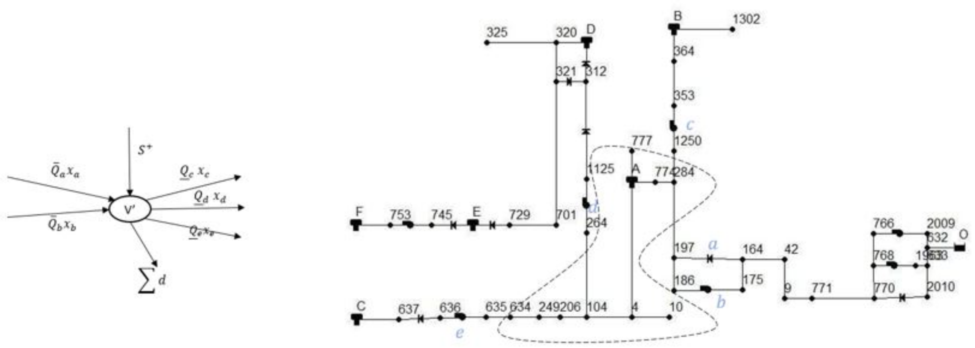

FIG. 2 – The flow cutset-based inequality and a supernode in the *Poormond* network.

inequalities [1]. The definition of cover set with respect to (8) deviates from the original one for knapsack inequalities due to the change of sign and the presence of negative coefficients. We handle this by taking the complement $\bar{x}_{at} = 1 - x_{at}$, then a cover set $C = C^- \cup C^+ \subset (A_v^- \cup A_v^+) \times \mathbb{T}'$ for (8) satisfies $\lambda_C = \sum_{t\in\mathbb{T}'} d_{vt} - \sum_{at\in C^-} \overline{Q}_{at} + \sum_{at\in C^+} \underline{Q}_{at} > 0$. At $t' = 0$, the level in tank j is fixed then variable $h_{jt'}$ vanishes in (8), otherwise for the cover inequality to be valid, we consider intervals $\mathbb{T}'$ such that $\underline{H}_{j(t'+\tau+1)} \geq \underline{H}_{jt'}$, then $(h_{jt'} - \underline{H}_{jt'}) \geq (h_{jt'} - \underline{H}_{j(t'+\tau+1)})^+ \geq 0$, and we get :

$$\sum_{at\in C^-} \min\{\overline{Q}_{at}, \lambda_C\} x_{at} + \sum_{at\in C^+} \min\{\underline{Q}_{at}, \lambda_C\}(1 - x_{at}) + \frac{1}{\sigma_j}(h_{jt'} - \underline{H}_{jt'}) \geq \lambda_C. \tag{9}$$

The cover inequalities can be further strengthened by lifting with variables in (8) not in cover C, i.e. in the complement $C_\top = C_\top^- \cup C_\top^+ = (A_v^- \cup A_v^+) \times \mathbb{T}' \setminus C$. The multipliers of variables can be derived either via superadditivity [1] or via Mixed integer rounding [7]. For instance, the lifted cover inequality via MIR is represented as :

$$\sum_{at\in C^-}\min\{\overline{Q}_{at},\lambda_C\}x_{at}+\sum_{at\in C^+}\min\{\underline{Q}_{at},\lambda_C\}(1-x_{at})+\frac{1}{\sigma_j}(h_{jt'}-\underline{H}_{jt'})\geq \lambda_C\big(1+\sum_{at\in C^-_{\top}}\Phi_{MIR}(\overline{Q}_{at})(1-x_{at})+\sum_{at\in C^+_{\top}}\Phi_{MIR}(\underline{Q}_{at})x_{at}\big) \quad (10)$$

where $\Phi_{MIR}(Q_{at})=\lfloor\frac{Q_{at}}{Q^*}\rfloor+\frac{(Q_{at}/Q^*-\lfloor Q_{at}/Q^*\rfloor-1+\lambda_C/Q^*)^+}{\lambda_C/Q^*}$ with $Q^*=\max_{at\in C_\top}\{Q_{at}\}$ and $Q^*>\lambda_C$.

We can take leverage from the dependencies of the arcs and make the inequalities tighter. For instance, if the activity of the arc a_2 is dependent on the activity of the arc a_1 and they are parallel, then instead of using the absolute capacities Q_{a_1} and Q_{a_2}, which will be a loose underestimator or overestimator of the flow variable, we can consider two different capacities derived from possible combinations. The next issue regarding these inequalities is how to select cover inequalities. Given the topology of the network, the number of possible combinations of the elements in the network graph to generate the cutset-based inequalities are limited. Since the inequalities introduced in 8 are valid whenever the time steps are consecutive, the number of subsets for such inequalities is restricted too. One major issue regarding the flow cutset-based inequalities in this framework is the presence of continuous variables, which makes the lifted inequalities looser (note that lifted minimal cover inequalities[1] without continuous variables are theoretically face-defining). To mitigate its effect, we propose to generate the inequality at time t when the water level in tank j' is close to its lower bound in the solution of the LP relaxation. According to the mentioned consideration, we adopt the separation problem introduced by [6] to select cover inequalities.

5 Computational Experiments

We assess the effect of bound tightening and cut generation at the preprocessing stage by defining three formulations : without preprocessing (B0), with bound tightening (B1), and with bound tightening and cutting planes (B2) on the global optimization of the MILP relaxation. We consider groups of 5 instances from the literature, for different time horizons $T=12,24,48$ and for different networks : *Simple Network* (S) consists of 3 pumps, 1 tank, and 2 pipes, and the realistic *Poormond* network (P) consists of 7 pumps, 4 valves, 5 tanks, and 43 pipes. To have a fair comparison between formulations, experiments for B1 and B2 formulations are run for 1 hour while we let it run over B0 for one additional hour (the most time-consuming bound tightening takes less than 1 hour). The preprocessing Code and experiments are available on github `https://github.com/sofdem/gopslpnlpbb/tree/roadef`. Table 1 illustrates the optimization performance with B0, B1, and B2 formulations over the benchmark.

In the smallest group S24, all formulations are able to solve the 5 instances in a few seconds. By increasing the time horizon to 48, formulation B0 proves optimality for only one instance, B1 for 3 instances, and B2 for all 5 instances. For the larger network P, formulation B0 cannot even compute one feasible solution within two hours. With bound tightening, B1 computes feasible solutions for all instances and proves optimality once. With the additional valid inequalities, B2 solves all instances to optimality. For P24 and P48, preprocessing helps to shrink the mean optimality gap from, respectively, 4% and 3% to roughly 2%. Furthermore, preprocessing B2 provides more feasible solutions during the branch and check algorithm. The difference reaches to almost two times higher in P24 with B2 formulation with respect to B0. Besides, it reduces the time to compute a first feasible solution, for P24 the average time is reduced from 693s in B0 to 172s in B1 and 104s in B2. Similar trend can be observed in P48.

6 Conclusions

The problem-specific bound tightening and cutting generation at the preprocessing stage have resulted in a noticeable improvement in the optimization of the pump scheduling problem, yet this preprocessing could be costly. The main ideas introduced in this paper, that is relaxing the time intervals and focusing on some deemed crucial elements and subgraphs over the network, would generalize

		S24	S48	P12	P24	P48
	#feas	5	5	0	4	5
B0	#opt	5	1	0	0	0
	avg-gap	0%	0.5%	inf	4.1%	3.2%
	#feas	5	5	5	5	5
B1	#opt	5	3	1	0	0
	avg-gap	0%	0.2%	2.3%	2.8%	2.8%
	#feas	5	5	5	5	5
B2	#opt	5	5	5	0	0
	avg-gap	0%	0%	0%	2.2%	2.1%

TAB. 1 – Experimental comparison of formulations B0 (no preprocessing), B1 (+ OBBT) and B2 (+cuts) : #feas : number of instances for which at least 1 feasible solution is computed, #opt : number of optimality proofs, avg-gap : average optimality gap.

the approach for remarkably larger networks. The detection of crucial time instants and elements could be controlled by a heuristic or a learning algorithm based on historical data to make the preprocessing stage more effective and efficient. Due to the resemblance of the mathematical formulation of water and gas networks, some ideas can be interchangeably adopted [5, 9].

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