Bilevel Optimization and ReLU Neural Nets for Control Optimization of Water Distribution Networks

Master’s Dissertation Proposal

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Abstract

This research project will address the challenges faced in the optimization and control of water distribution networks (WDNs) through modeling, implementation and testing of optimization strategies. The efficient distribution of drinking water is crucial to the functioning of communities around the world, and small improvements can have a significant impact on public services and people's quality of life. The project aims to develop improved WDN models in mixed-integer nonlinear programming (MINLP) and implement them in the Julia programming language, together with the JuMP algebraic modeling language. A central part of the project is the application of bilevel optimization to combine the strategy and operational level of the WDN management, and the integration of rectified linear neural networks (ReLU) to represent pumps with variable speed, aiming for a more accurate and efficient representation of these critical components of WDNs. The project methodology is divided into several stages, including literature review, model development and training, implementation in Julia/JuMP, and testing and validation of the proposed models. The effectiveness of the developed solutions will be evaluated by comparison with high-fidelity simulations using the EPANET software, a simulator widely used for modeling WDNs. Expected results include accurate and efficient WDN models, implemented in Julia/JuMP, and a comprehensive analysis of the effectiveness of these models in optimizing and controlling water distribution networks using bilevel optimization. Furthermore, the project is expected to advance the state-of-the-art in modeling and operation of WDN, and also to the practice by delivering precise and efficient optimization solutions to water distribution companies, improving efficiency and sustainability of their water network.

Key-words: Water distribution networks, MINLP, MILP, Bilevel Programming, ReLU neural networks, Julia, JuMP

1) Introduction

The distribution of drinking water is essential for everyone, practically anywhere on the planet. Water distribution networks (WDNs) around the world require significant resources for their operation. Any small improvement has the potential to positively impact public water services, ultimately benefiting people.

Improving complex systems like WDNs, which are often extensive and consist of several different components, takes work. On the one hand, improving individual components often requires replacing old technologies, a task that depends significantly on financial resources. On the other hand, systemic improvements, based on WDN models capable of predicting the impact of a change and directing actions, have the potential to provide the best returns.

A natural path to improvement is to reduce costs or increase the level of service. Among the various WDN operating costs, electricity for water utilities stands out. Approximately 4% of electricity use in the United States is attributed to water and wastewater supply, transportation, and treatment. For a typical surface water utility, 80% to 85% of its overall operating cost comes from pumping in the distribution system (Denig-Chakroff, 2008).

Increasing efficiency is the most direct step to reducing electrical energy consumption in pumping systems. Many options are available: first, on the individual component side, replacing inefficient motors and installing speed controllers; second, on the systemic side, although less advanced, using operational controllers, that is, a system that allows collecting measurements and controlling pumps and valves remotely; finally, on the advanced systemic side, optimizing electrical energy management and the use of pumps.

Optimizing electrical energy management in WDNs involves pumping and storing water in tanks during periods when energy costs are lower and, conversely, stopping pumping and distributing the stored water to consumers when the energy price is higher. This process must ensure minimum tank water inventories and adequate pressure at consumer sites. The efficiency of the pumps depends on the inlet and outlet pressures, the state of the WDN, and the rotor speed. Optimizing its operation requires pumping at a specific speed at the right time to achieve the highest possible efficiency.

Operational optimization generally focuses on minimizing operational costs while maintaining an acceptable level of service to customers, considering system constraints and legal regulations (Brdys; Ulanicki, 1994). These goals often conflict. Attempts to minimize operational costs can make the system more vulnerable and less capable of responding to abnormalities, thus reducing the level of service (Jowitt et al., 1988).

Given the interrelationship between optimizing electrical energy management and optimizing pump usage, these tasks should ideally work in a coordinated manner. Service quality policies, legal regulations, and the interconnected nature of WDN hydraulic behavior require accurate prediction of the state of WDN within certain limits. Addressing inseparable optimization objectives within tight constraints implies that the WDN model for optimization is highly accurate.

To address this challenge, Zyl (2001) proposed a Mixed-Integer Nonlinear Programming MINLP) formulation based on differential equations that describe the dynamics of systems with on/off pumps, tanks, and pipes designed to minimize pump operating costs. Due to their complexity, the solutions for the proposed instances, which later became benchmarks, were obtained with the help of genetic algorithms (Zyl; Savic; Walters, 2004) instead of solving the model directly. Penalties for volume deficit in tanks were imposed at the end of the simulation period and penalties for violating the limit on the number of pump switches. Figure 1 depicts the baseline WDN introduced by Zyl (2001).

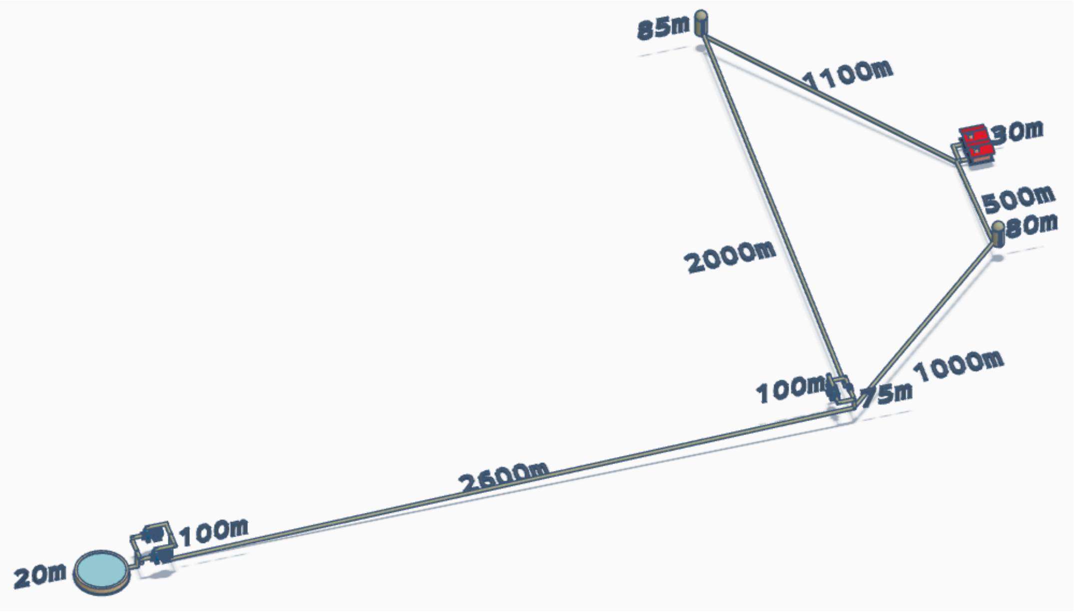

Figure 1. Water distribution network introduced by Zyl (2001)

Ghaddar et al. (2015) proposed a static MINLP formulation to minimize pump operating costs by applying a Lagrangian decomposition that divides the original problem into smaller problems. Significant improvements were achieved using a simulation-based search algorithm. These authors demonstrated that the Lagrangian decomposition outperforms a piecewise-linear approximation. The proposed model considers on/off pumps, tanks, and pipes and includes several constraints, such as the upper limit for pipe flows and the condition that the pump must be on for water to flow in the corresponding pipe. Recently, Vieira et al. (2020) applied a piecewise linearization in a more complete RDA model that considers full tanks.

By observing the accentuated rate of new publications in the area, the question naturally arises about the accuracy of the WDN models presented. One of the best places for this assessment is EPANET, a free WDN simulation tool developed by the United States Environmental Protection Agency (EPA) (Rossman, 1994; Rossman, 2000). With more than 1,500 citations in journals and hundreds of thousands of downloads, EPANET is the reference software for the analysis and design of pressurized water distribution networks (Gómez et al., 2015).

When deeply analyzing the EPANET network model, it becomes evident that many works in the literature oversimplify the problem. They lack key elements in the WDN models: first, the variable speed pumps, which are among the most effective components for saving electricity consumption; second, pressure-actuated valves, which play a crucial role in managing network pressure and whose effects on the hydraulic behavior of WDNs should not be neglected. Figure 2 presents the EPANET model of the water distribution network introduced by Zyl (2001).

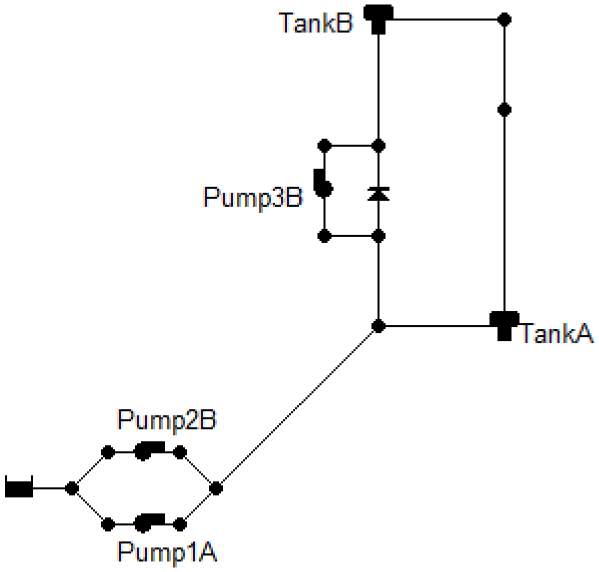

Figure 2. EPANET model of the water distribution network introduced by Zyl (2001)

Designing a complete MINLP formulation for WDNs and searching for an effective solution is a challenging research activity. On the other hand, the literature offers a wide range of techniques to solve these types of problems, such as the piecewise-linear MILP approximation (Vielma; Ahmed; Nehmauser, 2010), (Silva; Camponogara, 2014) and temporal decompositions such as the horizon- rolling

(Baker, 1977) and relax-and-fix (Dillenberger et al., 1994; Friske; Buriol; Camponogara, 2022).

2) Objectives

In the context of Luguesi's master's dissertation(2024), a complete and accurate mixed-integer nonlinear programming (MINLP) model was developed for WDNs, incorporating pressure safety valves (PSV), pressure relief valves (PRV), and variable speed pumps. This MINLP model covers the daily and hourly operation of WDNs, accounting for typical equipment such as unidirectional and bidirectional piping, various valves (PSV, PRV, and others), tanks, reservoirs, pressure and volume restrictions, and variable speed pumps. The model was validated by comparing behaviors simulated in EPANET. It was demonstrated that global optimization algorithms, available in solver packages such as SCIP (Bolusaniet al., 2024) and BARON, can find the global optimum for small but representative WDNs. A methodology based on piecewise linearization was employed to approximate the MINLP as a mixed-integer linear programming (MILP) problem. Although this approach provides an approximate solution for larger networks, even the MILP approximation was not solvable for practical networks within a reasonable time frame. The implementations were carried out using the algebraic language AMPL (Mathematical Modeling Programming Language) (Fourer; Gay; Kernighan, 2023) and the solvers Gubori and SCIP (Bolusaniet al., 2024).

Aiming to improve the MINLP model and implementation for optimized management of WDN, this research project has the following objectives:

1. Training ReLU Neural Networks (Grimstad & Andersson, 2019) as alternative models for variable speed pumps.
2. Implement ReLU networks in mixed-integer linear programming and replace nonlinear pump models in the MINLP problem that optimizes the operations in water distribution networks.
3. Implement the MINLP problem in the Julia programming language (Bezanson et al., 2017) and JuMP algebraic modeling language (Lubin et al., 2023).
4. Propose and implement a bilevel optimization strategy to explicitly divide strategic decisions (tank levels) from operational decisions (pump speeds), leveraging the efficiency of the bilevel decomposition (Colson; Marcotte; Savard, 2007), (Camponogara et al., 2021).
5. Test the efficiency of solving the MINLP problem for managing WDNs using the Julia and JuMP languages and the MILPs models of ReLU networks to represent pumps with variable speed.

6. Test the efficiency of solving the MINLP problem for managing WDNs as a bilevel program, comparing against standard strategies based on global optimization and the MILP approximation.

3) Methodology

This project will be executed in distinct stages, constituting a structured approach to ensure the efficient use of resources and systematic progress. The steps proposed for the research are:

1. *Literature Review and Scenario Preparation (Months 1-6):* During this phase, the team will conduct an in-depth and detailed review of existing literature on modeling water distribution networks. This review will deepen the understanding of existing work and also identify opportunities for scientific and technological advancement. In parallel with the literature review, data for WDN scenarios concerning scenarios from the literature and the EPANET simulator will be prepared. The scenarios will be relevant for simulation studies, training ReLU neural networks of variable speed pumps, proposing MINLP models, and designing bilevel optimization strategies for optimal operation of WDNs.
2. *Model Development and Training (Months 5-10):* In this step, the student will develop the variable speed pump proxy model using ReLU neural networks. The training process will be iterative, where model performance will be continually monitored, and adjustments will be made as necessary, including, but not limited to, the use of regularizations. This step will be crucial to optimize model performance, ensuring its effectiveness in the MILP representation of variable speed pumps using a reduced number of binary variables.
3. *Implementation in Julia/JuMP language (Months 6-10):* This stage involves the implementation in Julia/JuMP of the MILP models corresponding to ReLU neural networks trained to represent pumps with variable speed. Also, the implementation in Julia/JuMP of the MINLP model for optimizing the operation of water distribution networks, considering both the fundamental equations that model pumps and the proxy MILP models obtained from previously trained ReLU neural networks.
4. *Algorithm Design (Months 7-13):* Concerns the study and implementation of a bilevel programming strategy (Colson; Marcotte; Savard, 2007), (Camponogara et al., 2021), where the master problem deciding upon the tank levels over the prediction horizon, while the subproblem is split into several subproblems, one for each period (hour), concerning the operational decisions involving the activation and speed of pumps.

5. *Test and Validation (Months 9-16):* The testing phase will involve the use of the MINLP model in solving operational problems of representative WDNs based on the scenarios developed. The optimization results of the MINLP models, obtained with Julia/JuMP and optimization solvers, will be compared against the high-fidelity simulation generated with the EPANET simulator. Such trials will produce data to adjust and validate the models, as well as evaluate the gains obtained with optimized management of WDNs.
6. *Analysis and Documentation (Months 14-18):* In this phase, a comprehensive analysis of the results will be carried out, as well as documentation of the findings, insights and challenges faced. A detailed research report will be prepared, considering scenarios, proposed models, and results obtained. A scientific article will be prepared from the detailed report describing the models and results achieved. This documentation will be crucial for communicating the project results to the scientific community and other interested parties.
7. *Dissemination of Results (Months 15-18):* Finally, the results of the project will be shared with the academic and scientific community through the publication of articles in journals and presentations at conferences. It is planned to make the developed models available for use by the scientific community and water supply companies.

Throughout all stages, progress will be reviewed and readjusted regularly, fostering a collaborative environment to ensure adherence to the schedule. In addition to the advisors, the master's student can count on the invaluable support of other graduate students conducting research on related topics under the advisors' guidance, making this a true team effort.

4) Expected Results

The expected contribution of the master's dissertation are:

1. ReLU neural networks implemented in Python programming language, trained to model pumps with variable speed, having pump flow and speed as input variables and output and efficiency variables, discharge pressure (head), and the terms necessary for calculating the hourly operating cost of the pumps.
2. Analysis of the quality of the approximation obtained with ReLU network models of variable speed pumps.
3. A bilevel programming strategy for optimizing the operations of water distribution networks.
4. Implementation in Julia/JuMP and validation of the MINLP problem of the daily operation of water distribution networks based on the behavior of RDAs simulated with the EPANET software.
5. Implementation in Julia/JuMP of MILP models of ReLU networks of variable speed pumps, replacing the fundamental models based on physical laws in the MINLP problem, for optimizing WDN operations.

6. Implementation of bilevel programming strategies for WDN operations optimization.
7. Analysis of the efficiency of the bilevel programming approach implemented in Julia/JuMP language combined with MILP models of ReLU neural networks as "proxy" models of variable speed pumps.
8. Detailed technical reports and papers discussing the research, studies, and results obtained.

5) Project Execution

This project is likely to be successful. First, it will be based on theory, models, data, and implementations in AMPL developed within the scope of a master's dissertation (Luguesi, 2024). The language for the implementations is Julia with JuMP, which is modern and flexible. Optimization solvers to be used are open or made available free of charge for academic purposes.

This project will be conducted in the Department of Automation and Systems at UFSC, equipped with advanced laboratories and a wide range of technological resources, making it ideal for conducting research of this nature. The department has high-performance computers, a fundamental requirement for the computational analyzes that will be carried out in this project. These clusters provide the computing power needed to run complex simulations and large-scale data analysis, which is crucial to the success of this project. Solvers for optimization are also available.

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