Marcos Túlio Cirilo Dultra

TÍTULO DA TESE (MÁXIMO 130 CARACTERES) THESIS TITLE (MAX 130 CHARACTERS)

DOCUMENTO PROVISÓRIO



Marcos Túlio Cirilo Dultra

TÍTULO DA TESE (MÁXIMO 130 CARACTERES) THESIS TITLE (MAX 130 CHARACTERS)

Dissertação apresentada à Universidade de Aveiro para cumprimento dos requisitos necessários à obtenção do grau de Mestre em Engenharia de Computadores e Telemática, realizada sob a orientação científica do Doutor (Prof. Doutor António Gil D'Orey de Andrade Campos), Professor associado do Departamento de Engenharia Mecânica da Universidade de Aveiro, do Doutor (co-orientador), Professor auxiliar convidado do Departamento de Matemática da Universidade de Aveiro, da Doutora (co-orientadora), Professora associada c/ agregação do Departamento de Biologia da Universidade de Aveiro, e do Doutor (co-orientador), Professor auxiliar convidado do Departamento de Física da Universidade de Aveiro.

Texto Apoio financeiro do POCTI no âmbito do III Quadro Comunitário de Apoio.

(if applicable- Portuguese mandatory)

Texto Apoio financeiro da FCT e do FSE no âmbito do III Quadro Comunitário de Apoio.

(if applicable- Portuguese mandatory)

o júri / the jury

presidente / president

Prof. Doutor João Antunes da Silva professor associado da Universidade de Aveiro

vogais / examiners committee

Prof. Doutor João Antunes da Silva professor associado da Universidade de Aveiro

Prof. Doutor João Antunes da Silva professor associado da Universidade de Aveiro

Prof. Doutor João Antunes da Silva professor associado da Universidade de Aveiro

Prof. Doutor João Antunes da Silva professor associado da Universidade de Aveiro

Prof. Doutor João Antunes da Silva professor associado da Universidade de Aveiro



palavras-chave

texto livro, arquitetura, história, construção, materiais de construção, saber tradicional.

resumo

Um resumo é um pequeno apanhado de um trabalho mais longo (como uma tese, dissertação ou trabalho de pesquisa). O resumo relata de forma concisa os objetivos e resultados da sua pesquisa, para que os leitores saibam exatamente o que se aborda no seu documento. Embora a estrutura possa variar um pouco dependendo da sua área de estudo, o seu resumo deve descrever o propósito do seu trabalho, os métodos que você usou e as conclusões a que chegou. Uma maneira comum de estruturar um resumo é usar a estrutura IMRaD. Isso significa:

- Introdução
- Métodos
- Resultados
- · Discussão

Veja mais pormenores aqui:

https://www.scribbr.com/dissertation/abstract/

keywords

textbook, architecture, history, construction, construction materials, traditional knowledge.

abstract

An abstract is a short summary of a longer work (such as a thesis, dissertation or research paper).

The abstract concisely reports the aims and outcomes of your research, so that readers know exactly what your paper is about.

Although the structure may vary slightly depending on your discipline, your abstract should describe the purpose of your work, the methods you've used, and the conclusions you've drawn.

One common way to structure your abstract is to use the IMRaD structure. This stands for:

- Introduction
- Methods
- · Results
- Discussion

Check for more details here:

https://www.scribbr.com/dissertation/abstract/

acknowledgement of use of Al tools

Recognition of the use of generative Artificial Intelligence technologies and tools, software and other support tools.

I acknowledge the use of [insert AI system(s) and link] to [specific use of generative artificial intelligence or other tasks]. I acknowledge the use of [software, codes or platforms] to [specific use software, codes or platforms or to other tasks].

Example 1: I acknowledge the use of ChatGPT 3.5 (Open AI, https://chat.openai.com) to summarise the initial notes and to proofread the final draft and the use of Office365 (Microsoft, https://www.office.com) for text writing and productivity.

Example 2: No content generated by AI technologies has been used in this Thesis.

Contents

List of Figures

List of Tables

Glossário

Introduction

1.1 Background

A finite and essential resource for human existence is water. Because it is of utmost importance, effective control and monitoring of its use are required. Moreover, it is necessary to consider not only its usage but also the energy and costs related to supplying it to the population.

Nowadays, various technologies can be employed to optimize water usage and reduce costs, such as Machine Learning algorithms to predict consumption, the use of sensors to monitor it, hydraulic model calibration, among others.

In WSS (Water Supply Systems), cost optimization is challenging because several factors must be considered, including network topology, water demand, and reservoir location. Another difficulty stems from data uncertainty, as in many cases, the collected data are inaccurate or incomplete.

In the computational field, the complexity of calculations or the lack of source-generated data are no longer as significant hurdles as they were a few years ago. With IoT (Internet of Things) and cloud computing, it is possible to collect and process vast amounts of data in real time. This dataset (Big Data) can be used to train Machine Learning algorithms and optimize costs in WSS.

Given these challenges, technology is an ally in addressing the various aspects involved.

1.2 Aim

In the literature, there are implementations that use various Machine Learning algorithms to simulate and optimize costs in water supply systems.

The goal of this article is to employ the DC3 (Deep Constraint Completion and Correction) algorithm as a new method for simulation and optimization and to compare the results obtained with existing algorithms, using the Fontinha and Ronqueira water supply systems as data sources.

1.3 Reading guide

This work is structured into 5 chapters:

- Chapter 1: Introduction to the theme, addressing its importance, the problems to be solved, as well as a possible solution, the aim of the work, and the structure of the dissertation.
- Chapter 2: Literature review. It includes hydraulic simulation using the EPANET tool, the use of Deep Learning in water supply systems, optimization, hard constraints, and the optimization process.
- Chapter 3: Methodology used for cost optimization in water supply systems with the DC3 (Deep constraints correction and completion) algorithm.
- Chapter 4: Implementation of the techniques and interpretation of the results obtained in each of the observed case studies.
- Chapter 5: Presentation of conclusions summarizing all the work carried out and suggestions for future studies.

State of the Art

2.1 Hydraulic Simulation

Currently, there are several hydraulic simulators on the market used to model water supply systems, such as EPANET, WaterGEMS, and WaterCAD. Simulation provides quick and accurate solutions to differential algebraic equations for developing a mathematical representation of a water supply system[1]. EPANET is one of the most recognized applications in water distribution[2], widely used and quite successful[3] for over 20 years[4], and this tool will be used to obtain the data needed for optimization.

2.2 Deep Leaning

2.2.1 Neural network

The main concept of neural networks (NN) was proposed and introduced as a mathematical model of an artificial neuron in 1943[5].

Basics components of a neural network architecture are neurons, activations, biases, weight and layers - in order to define the multilayer perceptron (MLP) model.[5]

INCLUIR FORMULA The most basic component of the neural network is the neuron and consists of two simple operations: the preactivation zi of a neuron is a linear aggregation of incoming signals, where each signal is weighted by Wij and biased by bi. Each neuron then fires or not according to the weighted and biased evidence, according to the values of the preactivation zi, and produces an activation.

The scalar-valued function is called the activation function and acts independently on each component of the preactivation vector.

Taken together, these neurons form a layer.[6]

For the activation function, the most common are the sigmoid, tanh, sin, linear, ReLU, GELU and other functions.

2.2.2 Deep Learning

Deep learning is a name for a specific class of artificial neural networks, which in turn are a special class of machine learning algorithms, applicable to natural language processing, computer vision, robotics and many more.[7]

Traditional Machine Learning algorithms use handwritten feature extraction to train algorithms, while Deep Learning algorithms use modern techniques to extract these features in an automatic fashion.[5]

It has been demonstrated unequivocally that multilayered artificial neural architectures can learn complex, non-linear functional mappings, given sufficient computational resources and training data. Importantly, unlike more traditional approaches, their results scale with training data. [8]

Deep learning provides a black-box method to learn from complex, high-dimensional data in order to infer robust and scalable insights, minimizing the degree of manual work required[5]. A feature that sets deep learning apart from its broader field of machine learning is the use of multilayer models that lead to a higher-level representation of the underlying data sources[8].

Neural networks are capable of learning—by changing the distribution of weights it is possible to approximate a function representative of the patterns in the input. The key idea is to re-stimulate the black-box using new excitation (data) until a sufficiently well-structured representation is achieved. Each stimulation redistributes the neural weights a little bit—hopefully in the right direction, given the learning algorithm involved is appropriate for use, until the error inapproximation with respect to some well-defined metric below a practitioner-defined lower bound. Learning then, is the aggregation of avariable length of causal chains of neural computations[9] seeking to approximate a certain pattern recognition task through linear/nonlinear modulation of the activation of the neurons across the architecture.

The use of Deep Leaening has grown tremendously in the last few years with the rise of GPUs, big data, cloud providers such as Amazon Web Services (AWS), Microsoft Azure and Google Cloud, and frameworks such as PyTorch, Keras, TensorFlow and many others. In addition to this, large companies share algorithms trained on huge datasets, thus helping startups to build state-of-the-art systems on several use cases with little effort.[5]

2.2.3 Deep Learning in WSS

The increasing demand for efficiency and sustainability in water supply systems has driven the use of Machine Learning and Deep Learning as innovative tools for optimization, monitoring, and control of these networks. With data obtained from tools like EPANET, it is possible to train machine learning models to predict system behavior and optimize resource usage.

There are several papers addressing the use of Deep Learning in water supply and distribution systems to predict anomaly detection[10], predict pressure in the water supply network[11], detect leaks[12], and smart scheduling to turn the pump on and off according to real-time monitoring[13], among others.

2.3 Optimization in WSS

Optimization is applied in many systems and situations, thus making it an important paradigm in technology. When we try to optimize, we either minimize (resource consumption, cost) or maximize (profit, system performance)[14].

In a more technical sense, optimization is said to be the process of maximizing or minimizing the required objective function while satisfying certain constraints.[15]

Water supply pumping stations are an indispensable element of any water supply system. They not only provide the water supply to each container but also the necessary pressure in the water supply network for firefighting purposes. The cost of energy is one of the most important components of the price of treated water.[16]

The main objective for optimization is the operational cost, which encompasses the cost of electric power and pump maintenance.[17] Pumping systems consume the largest amount of energy in water supply systems, generally accounting for more than 80% of the total energy consumption.[18]

Energy cost optimization in water supply systems can be achieved through several measures, such as pump replacement, changes in pumping station operations, pipe system modernization, computational modeling of network operation changes, and the selection of solutions that ensure the best economic and technical effects.[16]

WSS optimization has numerous applications, but it is crucial to highlight the importance of pump scheduling optimization due to the considerable energy consumption associated with this essential WSS component (Cost efficiency in water supply systems: An applied review on optimization models for the pump scheduling problem)

Pumping systems have significant potential for energy efficiency improvements. In many cases, operations optimization considers fixed pump speed, and cost savings can be obtained by using the variation in electricity tariff rates throughout the day.[18]

Hourly variations in water demand during the day are much higher compared to the average daily demand. For a household consumer, water demand is higher during morning and evening hours than midday. During peak hours, energy costs can be 2 to 3 times more expensive than during off-peak hours.

A technical solution for this reduction may involve decreasing pumping power (even stopping pumps if possible) during peak hours, along with extensive delivery outside these hours. Consequently, distribution systems must be equipped with storage tanks.

2.3.1 Mathematical formulation

Mathematical optimization models are mathematical representations of real-world problems that aim to find the best solution among a set of available alternatives.[19]

$$minimise f(x) (2.1)$$

subject to:
$$g(x) \le 0$$
 (2.2)

$$h(x) = 0 (2.3)$$

Where x represents a vector of decision variables or control variables that effect the operation of the water system. The decision variables x might represent pump flow rates, valve settings, reservoir release, or the allocation of the water resources over time. f(x) is the objective function, and g(x) is the inequality constraints, and h(x) is the equality constraints.

In operational water management, inequality constraints(??) can specify ranges of feasible system states, such as the capacity limits of pumps and turbines or the upper and lower volume limits of a reservoir. Equality constraints (??) are often represented by system equations, such as a water balance equation. A constraint violation makes the solution infeasible.

Due to its complexity, there are some common optimization problems that are fundamental for our understanding:

- Linearity and convexity: A linear optimization problem has a linear objective function and constraints, with the optimal solution always at a corner of the feasible region. This allows for efficient solution methods. Convex functions have a single minimum and no local minima, making them easier to minimize. A problem is convex if the objective function and inequality constraints are convex, while equality constraints are affine transformations.
- Continuous and discrete problems: A continuous problem has variables that can take
 any real value within a range, while a discrete problem includes variables like integers
 or Booleans with a finite set of values. Discrete variables are used for on/off decisions
 or to approximate nonlinear functions piecewise. These problems are generally harder
 to solve than continuous ones, so minimizing discrete variables balances model accuracy
 and computation time.
- Linear programming: Linear programming (LP) is used for problems with linear objectives and constraints, solving them efficiently with polynomial runtime. In water management, reservoir optimization is a common LP application. To leverage LP's advantages, models are often linearized, even at the cost of accuracy. This can be done through linear approximations or piecewise linear methods, commonly used in model predictive control (MPC), where frequent updates help mitigate accuracy loss.
- Nonlinear problems: Nonlinear problems occur when any part of the optimization (objective or constraints) is nonlinear. They may be convex or non-convex, and can be continuous or discrete. Generally, convex continuous problems are less complex to solve than non-convex discrete ones.
- Integer linear programming: Integer linear programming (ILP), or mixed integer programming (MIP), is used when some or all decision variables are restricted to discrete values. MIP is commonly applied in hydropower scheduling and pumping optimization. It is also useful for solving piecewise linear approximations of nonlinear equations.

2.4 Hard Constraints

Hard constraints is a term used to check whether certain properties are satisfied for solving optimization problems. [20] They are like non-negotiable rules.

Meeting constraints corresponds to applying operational safety limits and adhering to physical laws, which is of great importance.[21]

Gradient-based learning algorithms allow optimizing network parameters to approximate any desired model. However, despite the existence of several advanced optimization algorithms, the issue of imposing strict equality constraints during training has not been sufficiently addressed.[22]

Applying traditional solvers for general constrained optimization, such as SQP[23], to neural networks can be non-trivial. Since traditional methods express constraints as a function of learnable parameters, this formulation becomes extremely high-dimensional, non-linear, and non-convex in the context of neural networks.[22]

Water supply system operations are constrained by minimum pressure requirements; capacity limitations imposed by pumps, pipes, and tanks; and a set of hydraulic constraints. These hydraulic constraints give rise to complex mixed-integer and non-linear formulations. The first class of methods explicitly imposes pressure and capacity constraints, while hydraulic constraints are implicitly included through water network simulation tools, such as EPANET.[24]

2.5 Optimization Process

2.5.1 Mathematical Formulation

2.5.2 Optimization Methods

The new methodology combines the use of trigger levels with pump scheduling to optimize pump operations by maximizing off-peak tariff period pumping and minimizing pumping head.

Methodology

3.1 Pump Scheduling Problem

Abordagens de otimização: B-GA, RC-SLSQP e DC-SLSQP (Cost efficiency in water supply systems: An applied review on optimization models for the pump scheduling problem) Como foi feita a otimização (gradiente descendente / equações)

- 3.2 Presenting DC3 Algorithm
- 3.3 Algorithm architecture
- 3.4 Exemplos com grafico x1, x2

Results

4.1 Case study 1

Introdução

A short description of the chapter.

A memorable quote can also be used.

5.1 ACRÓNIMOS

Primeira e seguintes referências: **h2o!** (**h2o!**), **h2o!** Plural, acrónimo expandido e curto: **h2o!**s, **h2o!**, **h2o!**

Com citação¹: adsl! (adsl!), adsl!

5.2 Fontes

- Tiny
- Scriptsize
- Footnotes
- Small
- Normal
- large
- Large
- LARGE
- huge
- . Huge

5.3 Unidades

Utilizando o pacote $\mathtt{siunitx}$ é possível utilizar unidades do Sistema Internacional. Exemplo: a aceleração da gravidade é de $9.8\,\mathrm{m\,s^{-2}}$ e um ficheiro ocupa 1 MiB.

¹Necessária entrada na bibliografia

5.4 Code Blocks

Uma listagem pode ser apresentada com o ambiente listing, que é um float (objeto flutuante, tal como uma figura ou uma tabela).

A listagem em Código ?? mostra um exemplo em C.

Código 1: This caption appears below the code.

5.5 Citações

Algumas formas distintas de citar:

• Apenas referência: [1]

• Apenas data: 2015

• Apenas ano: 2015

• Apenas autor: Paluszczyszyn et al.

• Apenas editor:organization

• Autor e referência:Paluszczyszyn et al. [1]

Exemplos

A short description of the chapter.

A memorable quote can also be used.

6.1 Acrónimos

Primeira e seguintes referências: h2o!, h2o!

Plural, acrónimo expandido e curto: h2o!s, h2o!, h2o!

Com citação¹: adsl!, adsl!

6.2 Fontes

- Tiny
- Scriptsize
- Footnotes
- Small
- Normal
- large
- Large
- LARGE
- huge
- . Huge

6.3 Unidades

Utilizando o pacote siunitx é possível utilizar unidades do Sistema Internacional. Exemplo: a aceleração da gravidade é de $9.8\,\mathrm{m\,s^{-2}}$ e um ficheiro ocupa 1 MiB.

¹Necessária entrada na bibliografia

6.4 Code Blocks

Uma listagem pode ser apresentada com o ambiente listing, que é um float (objeto flutuante, tal como uma figura ou uma tabela).

A listagem em Código ?? mostra um exemplo em C.

Código 2: This caption appears below the code.

6.5 CITAÇÕES

Algumas formas distintas de citar:

• Apenas referência: [17]

• Apenas data: Apr. 2013

• Apenas ano: 2013

• Apenas autor: Folorunso and Ismail

• Apenas editor:organization

• Autor e referência:Folorunso and Ismail [17]

Bibiliography

- [1] D. Paluszczyszyn, P. Skworcow, and B. Ulanicki, "Modelling and simulation of water distribution systems with quantised state system methods," *Procedia Engineering*, vol. 119, pp. 554–563, 2015, Computing and Control for the Water Industry (CCWI2015) Sharing the best practice in water management, ISSN: 1877-7058. DOI: https://doi.org/10.1016/j.proeng.2015.08.908. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S1877705815025783.
- [2] L. A. Rossman, *Epanet user's manual. version 2.2*, EPA, Risk Reduction Engineering Laboratory. Office of Research and Development. Environmental Protection Agency, 2000.
- [3] M. Davis, R. Janke, and T. Taxon, Mass imbalances in epanet water-quality simulations, Apr. 2018. DOI: 10.5194/dwes-11-25-2018.
- [4] M. Hervás, F. Martínez-Alzamora, P. Conejos, and J. C. Alonso, Advantages of the event method for the simulation of water quality in pressurised water systems, 2024. [Online]. Available: https://www.mdpi.com/2073-4441/16/4/599.
- [5] V. Subramanian, Deep Learning with PyTorch, P. Publishing, Ed. 2018, ISBN: 978-78862-433-6.
- [6] D. A. Roberts, S. Yaida, and B. Hanin, The Principles of Deep Learning Theory: An Effective Theory Approach to Understanding Neural Networks. Cambridge University Press, May 2022, ISBN: 9781316519332. DOI: 10.1017/9781009023405. [Online]. Available: http://dx.doi.org/10.1017/9781009023405.
- [7] S. Skansi, Introduction to Deep Learning, Springer, Ed. 2018.
- [8] S. Sengupta, S. Basak, P. Saikia, et al., "A review of deep learning with special emphasis on architectures, applications and recent trends," Knowledge-Based Systems, vol. 194, p. 105 596, 2020, ISSN: 0950-7051. DOI: https://doi.org/10.1016/j.knosys.2020.105596. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S095070512030071X.
- [9] J. Schmidhuber, "Deep learning in neural networks: An overview," Neural Networks, vol. 61, pp. 85-117, 2015, ISSN: 0893-6080. DOI: https://doi.org/10.1016/j.neunet.2014.09.003. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0893608014002135.
- [10] K. Qian, J. Jiang, Y. Ding, and S. Yang, Deep learning based anomaly detection in water distribution systems, 2020. DOI: 10.1109/ICNSC48988.2020.9238099.
- [11] S. Zhao, Z. Li, F. Wang, B. Sun, L. Li, and H. Zhang, Pressure prediction of water supply network based on 1dcnn-gru-multi-head attention, 2024. [Online]. Available: https://doi.org/10.2166/ws.2024.169.
- [12] H. Yu, S. Lin, H. Zhou, X. Weng, S. Chu, and T. Yu, Leak detection in water distribution networks based on deep learning and kriging interpolation method, 2024. [Online]. Available: https://doi.org/10.2166/aqua.2024.184.
- [13] Z. Pu, M. Chen, X. Ji, et al., Intelligent real-time scheduling of water supply network based on deep learning, Nov. 2023. DOI: 10.2166/aqua.2023.134.

- [14] O. Awe, S. Okolie, and O. Fayomi, "Optimization of water distribution systems: A review," *Journal of Physics: Conference Series*, vol. 1378, no. 2, p. 022068, 2019. DOI: 10.1088/1742-6596/1378/2/022068. [Online]. Available: https://dx.doi.org/10.1088/1742-6596/1378/2/022068.
- [15] A.Andrade-Campos, J.Dias-de-Oliveira, and J.Pinho-da-Cruz, Otimização não-linear em engenharia Cálculo estrutural e computacional multiescala. 2015, ISBN: 978-972-8480-35-6.
- [16] M. Świętochowska and I. Bartkowska, Optimization of energy consumption in the pumping station supplying two zones of the water supply system, 2022. [Online]. Available: https://www.mdpi.com/1996-1073/15/1/310.
- [17] T. Folorunso and F. S. Ismail, "Pump scheduling optimization model for water supply system using awga," Apr. 2013, pp. 12–17, ISBN: 978-1-4799-0209-5. DOI: 10.1109/ISCI.2013.6612367.
- [18] I. Sarbu, A study of energy optimisation of urban water distribution systems using potential elements, 2016. [Online]. Available: https://www.mdpi.com/2073-4441/8/12/593.
- [19] B. P. J. Becker, C. J. Jagtenberg, K. Horváth, A. Mitchell, and J. A. Rodríguez-Sarasty, "Optimization methods in water system operation," WIREs Water, vol. 11, no. 6, e1756, 2024. DOI: https://doi.org/10.1002/wat2.1756. eprint: https://wires.onlinelibrary.wiley.com/doi/pdf/10.1002/wat2.1756. [Online]. Available: https://wires.onlinelibrary.wiley.com/doi/abs/10.1002/wat2.1756.
- [20] Y. Min, A. Sonar, and N. Azizan, *Hard-constrained neural networks with universal approximation guarantees*, 2024. arXiv: 2410.10807 [cs.LG]. [Online]. Available: https://arxiv.org/abs/2410.10807.
- [21] S. Misra, L. Roald, and Y. Ng, Learning for constrained optimization: Identifying optimal active constraint sets, 2019. arXiv: 1802.09639 [math.OC]. [Online]. Available: https://arxiv.org/abs/1802.09639.
- [22] F. Zhong, K. Fogarty, P. Hanji, et al., Neural fields with hard constraints of arbitrary differential order, 2023. arXiv: 2306.08943 [cs.LG]. [Online]. Available: https://arxiv.org/abs/2306.08943.
- [23] J. Nocedal and S. J. Wright, Numerical optimization, 1999.
- [24] M. K. Singh and V. Kekatos, "Optimal scheduling of water distribution systems," *IEEE Transactions on Control of Network Systems*, vol. 7, no. 2, pp. 711–723, 2020. DOI: 10.1109/TCNS.2019.2939651.

Α

Additional content