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Comparison of Monte Carlo Algorithm, genetic algorithms and artificial neural networks for calibration of water supply networks using the epanet2toolkit

A comparison of three water network calibration algorithms was performed using the R epanet2toolkit library. This coupling makes it possible to explore EPANET's hydraulic simulation and evaluation potentials and data analysis in R, with the main result of the work being the comparison of three calibration methods. In the calibration process by the Monte Carlo Algorithm, 100,000 roughness values were randomly generated for each pipe section within the range of 0.008 to 0.09 and new pressure values were generated with these roughnesses, while the calibration by the Genetic Algorithms method was used the rpy2 package that allows the use of R in Python, having 10,000 generations per simulation with 5% chance of mutation and 50% chance of crossover, admitting a deviation of ± 2 m.c.a for each pressure and the reduction of the average error. Finally, the Neural Network calibration also used the rpy2 package, with the network demand defined as the input layer and the output layer as the roughness of the pipes and for the hidden layer the input layer plus four neurons was defined. The results showed that in the smallest network the best performance was obtained by the Genetic Algorithms, followed by Monte Carlo, while the Neural Network had the worst result, and in the most complex network the Neural Network results obtained the best result, followed by the Genetic Algorithms and Monte Carlo. Thus, the potential of using Neural Networks for the calibration of more complex networks is observed, as well as its use combined with optimization techniques for the operation of water distribution networks, taking care to avoid situations of overfitting or underfitting.

Keywords: Calibration; EPANET; Genetic Algorithms; Monte Carlo; Neural Networks.

Comparação do Algoritmo de Monte Carlo, algoritmos genéticos e redes neurais artificiais para calibração de redes de abastecimento de água utilizando o epanet2toolkit

Uma comparação de três algoritmos de calibração de redes de água foi realizada usando a biblioteca R epanet2toolkit. Este acoplamento permite explorar os potenciais de simulação e avaliação hidráulica do EPANET e análise de dados em R, sendo o principal resultado do trabalho a comparação de três métodos de calibração. No processo de calibração pelo Algoritmo de Monte Carlo foram gerados aleatoriamente 100.000 valores de rugosidade para cada seção de tubo na faixa de 0,008 a 0,09 e novos valores de pressão foram gerados com essas rugosidades, enquanto na calibração pelo método de Algoritmos Genéticos foi utilizado o pacote rpy2 que permite a utilização de R em Python, possuindo 10.000 gerações por simulação com 5% de chance de mutação e 50% de chance de cruzamento, admitindo um desvio de ± 2 m.c.a para cada pressão e a redução do erro médio. Por fim, a calibração da Rede Neural também utilizou o pacote rpy2, sendo a demanda da rede definida como a camada de entrada e a camada de saída como a rugosidade dos tubos e para a camada oculta foi definida a camada de entrada mais quatro neurônios. Os resultados mostraram que na menor rede o melhor desempenho foi obtido pelos Algoritmos Genéticos, seguido de Monte Carlo, enquanto a Rede Neural teve o pior resultado, e na rede mais complexa os resultados da Rede Neural obtiveram o melhor resultado, seguido pelo Algoritmos Genéticos e Monte Carlo. Assim, observa-se o potencial da utilização de Redes Neurais para a calibração de redes mais complexas, bem como a sua utilização aliada a técnicas de otimização para o funcionamento de redes de distribuição de água, tendo o cuidado de evitar situações de overfitting ou underfitting.

Palavras-chave: Calibração; EPANET; Algorítmos genéticos; Monte Carlo; Redes neurais.

Topic: **Engenharia de Recursos Hídricos**

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INTRODUCTION

Water resources are important for life and for all human activities. However, it is a limited resource, which has been decreasing due to the worsening of the water crisis and incorrect use. Thus, the study of water losses in distribution systems and ways to reduce them is relevant, as they cause great inconvenience to society and the environment. In Brazil, this volume of water lost in these systems is worrying. According to the loss report by Go Associados (2022), water losses in 2020 represented 7.2 billion m³ and if this volume were billed, it would generate revenue of approximately 14 billion reais.

Thus, the development of hydraulic simulation models is widely used to analyze the behavior of water in distribution systems, although its calibration is a great challenge due to the lack of data such as the state of the pipes, type of material used in the conduits and in some cases even their diameters. Thus, a correctly calibrated model can lead to a more reliable management level for water supply systems (ZANFEI et al., 2020). In this work, a brief survey of the application of calibration in academic works was carried out, with a time interval of seven years (2003 to 2022), presented in table 1.

Table 1: Timeline of network calibration applications.

Silva (2003)	Proposed a computational routine for the implementation of genetic algorithms for the purpose of calibrating real networks with significant leaks.	Goulart (2015)	Studied the improvement of some modules of the Calibration algorithm proposed by Silva (2003) and applied it to a real network in Cambuí-MG.
Savic et al. (2009)	They reviewed approaches to model calibration and considered future challenges and directions.	Santos (2016)	Studied the application and improvement of routine calibration of water distribution networks through calibration in a real case study in the city of São Lourenço-MG.
Santos et al. (2010)	Performed the calibration of a water distribution network in the city of Itajubá-MG using the model proposed by Silva (2003).	Do et al. (2016)	They presented an approach for calibrating demand multiplier factors under an inadequate condition, where the number of measurements is less than the number of parameter variables.
Tabesh et al. (2011)	They performed an optimization procedure that is designed to calibrate both types of hydraulic simulation models, demand-driven and pressure-dependent analyses, using genetic algorithms.	Diaz et al. (2017)	They researched calibration within a joint multi-period parameter and state estimation approach, where model parameters (ie roughness coefficients) and hydraulic variables must be calculated from measurements available at different times
Zhang et al. (2012)	They proposed a calibration model via a genetic algorithm coded together with a network solver (EPANET 2.0) to adjust the pipe roughness coefficients and nodal demand multipliers.	Minaee et al. (2019)	They proposed a sequential calibration methodology for any water quality model using specific estimates of the model's parameter range, which would help to better predict the water quality characteristics of the river.
Dini et al. (2013)	They researched a new method of calibrating water distribution networks via ant colony optimization algorithms (ACO) and compared the results with other existing methods.	Rathi et al (2020)	Studied the complexities and challenges involved in calibrating the city of Nagpur in India and describes the entire process of collecting data necessary for the calibration of the grid.
Abe (2014)	Proposed an automatic calibration system using artificial neural network techniques to improve the results of calibration systems.	Procel et al. (2021)	Modeled and analyzed three drinking water distribution networks and calibrated them with Epanet Calibrator Software, and compared the results with the calibration result of the Water GEMS hydraulic modeling software.
Vassiljev et al. (2015)	They studied whether the differences between real-time demand and typical demand can influence the calibration results, in addition to proposing some methods to minimize this influence.	Jun et al. (2022)	Researched the pipe roughness calibration of a water distribution system model, which focused on estimating input/output parameters of the model and analyzing various uncertainties (eg, model uncertainty) to improve models with parameters of best fit.

In this way, it was possible to observe tools and methods most used in the calibration of networks. Among the hydraulic simulation software, EPANET is one of those that has open and free code that performs hydraulic modeling and simulations, developed by the Environmental Protection Agency (EPA) of the United States, allowing to execute static and dynamic simulations of the hydraulic behavior in pressurized networks of water distribution, being the most used in the world for this purpose (ROSSMAN, 2009). It is a tool to support the analysis of distribution systems that assists in knowledge about the transport and destination of water for consumption (SPEDALETTI et al., 2022; ZAMAN et al., 2022; MENEPACE et al., 2020; SELA et al., 2019; ELIADES et al., 2016).

R is a computational language for statistical and graphic analysis, in addition to having a set of tools for data manipulation, calculations and graphical presentation through its RStudio integrated development environment, an environment that has more than 15 thousand packages and libraries with the most diverse applications that allow you to communicate with other software (SOUSA et al., 2020; SILVA, 2019; BISHWAL, 2017; PATEL et al., 2017; DIERAUER et al., 2017; HENNING et al., 2016).

The package epanet2toolkit is recently developed by Arandia et al. (2018) and was designed as a wrapper for EPANET, that is, its functions in R have the same name as the functions in EPANET when requested by the API (Programming Interface Applications) from Microsoft® Windows but differ in function contexts and return parameters. The working mechanism is the same for all functions: basically, the package exports the EPANET API functions to the R program, performs the analysis of the arguments, checks the error codes and returns the requested value (ARANDIA et al., 2018). The Monte Carlo method, despite being developed in the last century, is still considered one of the most advanced methods of simulation and optimization, since modern computing has allowed greater applicability in other problems. Essentially, this method consists of using random sampling to obtain numerical results (ERCOLANI et al., 2018; TOBISOVA et al., 2022). This model is used in several areas, also finding great application in water resources, including hydraulics. On the other hand, genetic algorithms, according to Silva (2003), are based on Darwin's theory of survival of the fittest, allowing the best solutions to advance and generate descending solutions over generations.

Artificial Neural Networks are computational techniques that present a mathematical model inspired by the neural structure of intelligent organisms and that acquire knowledge through experience, to which a large artificial neural network can have hundreds or thousands of processing units. For O'Reilly et al. (2018) artificial neural networks can be used to assist in efficient management of water supply systems. There are several types of artificial neural networks available, but the most commonly used are: Multi-layer Perceptrons (MLPs), Radial Basis Function (RBF), General Regression Neural Network (GRNN), Cascade Forward Networks (CFN) and Kohonen's self-organize maps (SOUND) (FARMAKI et al., 2010; WU et al., 2014).Studies have indicated that artificial neural networks are effective in predicting water resources, as they can replace conventional mathematical and statistical models or be associated with them (CHEN et al., 2019; SOUZA et al., 2010).

Alvisi et al. (2010) emphasize that the calibration process has a high degree of freedom, resulting in uncertainties, since the relationship between the number of monitored points, typically pressure and flow, and the number of variables is very low. A model is considered calibrated when the difference between simulated and real results reaches an acceptable level of error. Artificial Neural Networks (ANNs) have been widely used in conjunction with simulation and calibration models as they reduce degrees of freedom and help to provide more precision in the calibration process (MEIRELLES et al., 2017; SOUZA et al., 2021)

The importance of using computational modeling to analyze the behavior of water distribution networks was the main reason for the elaboration of this study that used three different models in order to compare them to find which one has the best result for the networks. used in the study, since the most reliable simulation possible of a water distribution network allows the use of optimization techniques, scenario prediction, simulation of adjustments and changes in the network in order to guarantee an operation closer to the optimal, reducing risks of water and energy losses in the system.

METHODOLOGY

The methodology used in the work was divided into six stages, as shown in Figure 1.

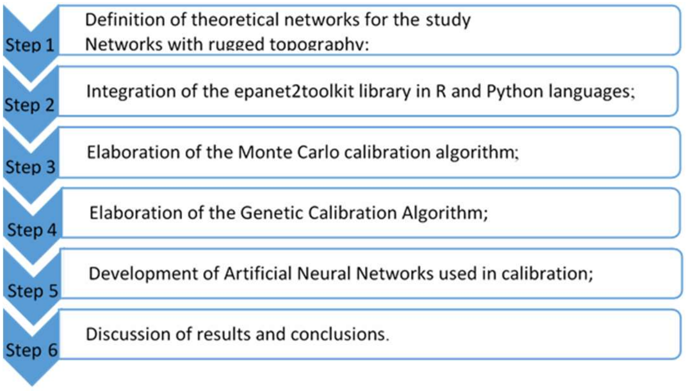

Figure 1: Flowchart of the study methodology steps.

Definition of theoretical water distribution networks for testing calibration models

In the second stage, theoretical networks of work were elaborated through the EPANET program. The first, simpler network is formed by a reservoir, eight nodes and eleven pipe sections, which were numbered sequentially according to the development of the route, whose details regarding consumption and elevation can be seen in Figure 1.

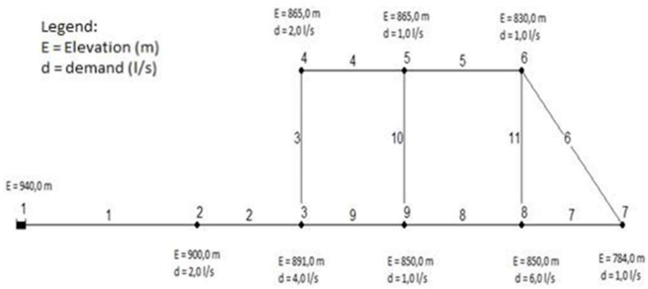

Figure 2: Simple network used in calibrations.

Details about the pipes, such as length, diameter and roughness are presented in Table 2, considering that for this network the universal equation was used.

Table 2: Length (meters), diameter (millimeters) and roughness of the.

Pipe Identifier	Length (m)	Diameter (mm)	Roughness
Pipe 1	1000	150	0.06
Pipe 2	800	100	0.06
Pipe 3	1000	75	0.06
Pipe 4	1000	100	0.06
Pipe 5	1000	100	0.06
Pipe 6	700	50	0.06
Pipe 7	900	50	0.06
Pipe 8	800	75	0.06
Pipe 9	800	75	0.06
Pipe 10	1000	150	0.06
Pipe 11	1000	75	0.06

The second network is more complex, having 1 fixed level reservoir, 29 nodes and 36 sections, also sequentially numbered and with the details regarding consumption and elevation can be seen in Figure 3.

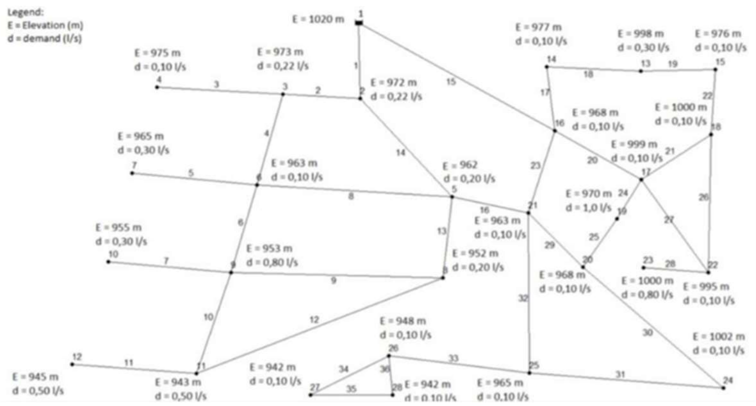

Figure 3: Complex network used in calibrations.

At the same way, details regarding pipes are presented in Table 3, considering for this network was used Hazen-Williams equation was used for calculations.

Table 3: Length (meters), diameter (millimeters) and roughness of the pipes.

Pipe Identifier	Length (m)	Diameter (mm)	Roughness
Pipe 1	1000	100	100
Pipe 2	1000	100	100
Pipe 3	1000	100	100
Pipe 4	1000	100	100
Pipe 5	1000	100	100
Pipe 6	1000	100	100
Pipe 7	1000	100	100
Pipe 8	1000	100	100
Pipe 9	1000	100	100
Pipe 10	1000	100	100
Pipe 11	1000	100	100
Pipe 12	1000	100	100
Pipe 13	1000	100	100
Pipe 14	1000	100	100
Pipe 15	1000	100	100
Pipe 16	1000	100	100
Pipe 17	1000	100	100
Pipe 18	1000	100	100
Pipe 19	1000	100	100
Pipe 20	1000	100	100

Pipe 21	1000	100	100
Pipe 22	1000	100	100
Pipe 23	1000	100	100
Pipe 24	1000	100	100
Pipe 25	1000	100	100
Pipe 26	1000	100	100
Pipe 27	1000	100	100
Pipe 28	1000	100	100
Pipe 29	1000	100	100
Pipe 30	1000	100	100
Pipe 31	1000	100	100
Pipe 32	1000	100	100
Pipe 33	1000	100	100
Pipe 34	1000	100	100
Pipe 35	1000	100	100
Pipe 36	1000	100	100
Pipe 37	1000	100	100

Both networks have an irregular topography in common, in order to simulate eventual distribution networks in mountainous regions such as the south of Minas Gerais, given that they represent a great challenge for their operation and also calibration, since they are expected to arise regions with excess or low pressure (SILVA et al., 2020).

Integration of epanet2toolkit package in R and Python

Thus, the integration between EPANET and R was carried out for the proposed networks. For this, the work of Arandia et al. (2018) was used as a basis for using the epanet2toolkit package, developed to apply the EPANET toolkit in R language. The package was designed as a wrapper for EPANET, that is, its functions in R have the same name as the functions in the EPANET when requested by the Microsoft® Windows application programming interface (API), but differ in function contexts and return parameters.

In addition to hydraulic simulations, epanet2toolkit addresses water quality simulations, both cases can be analyzed step by step or for extended periods, however the compatibility between the functions must be respected. Thus, the functions of epanet2toolkit can be used together with those available in R, triggering a range of dynamic applications, such as the creation of calibration systems defined in an optimization model or the elaboration of codes for demand forecasts through stochastic simulations (ARANDIA et al., 2018).

Elaboration of the Monte Carlo calibration algorithm

The model was elaborated in the R language so that the base scenario is initially run, that is, the distribution network is simulated in EPANET, using the Darcy-Weisbach equation for its solution, since the network it has sections with diameters below 2 inches, and it is not advisable to use Hazen-Williams. After the simulation and storage of the obtained pressures, the Monte Carlo method was applied to generate 100,000 roughnesses for each section, randomly. Afterwards, the network was simulated with the new roughnesses and the results were exported to an excel spreadsheet, as shown in the flowchart in Figure 4.

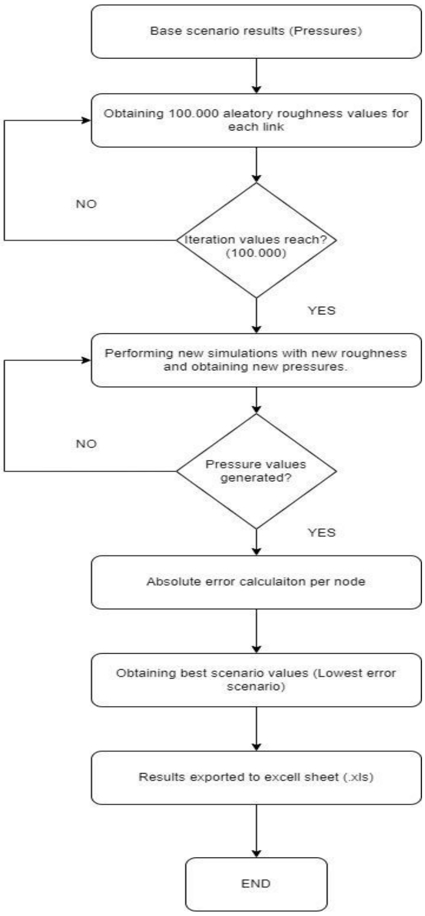

Figure 4: Flowchart of the Monte Carlo calibration algorithm.

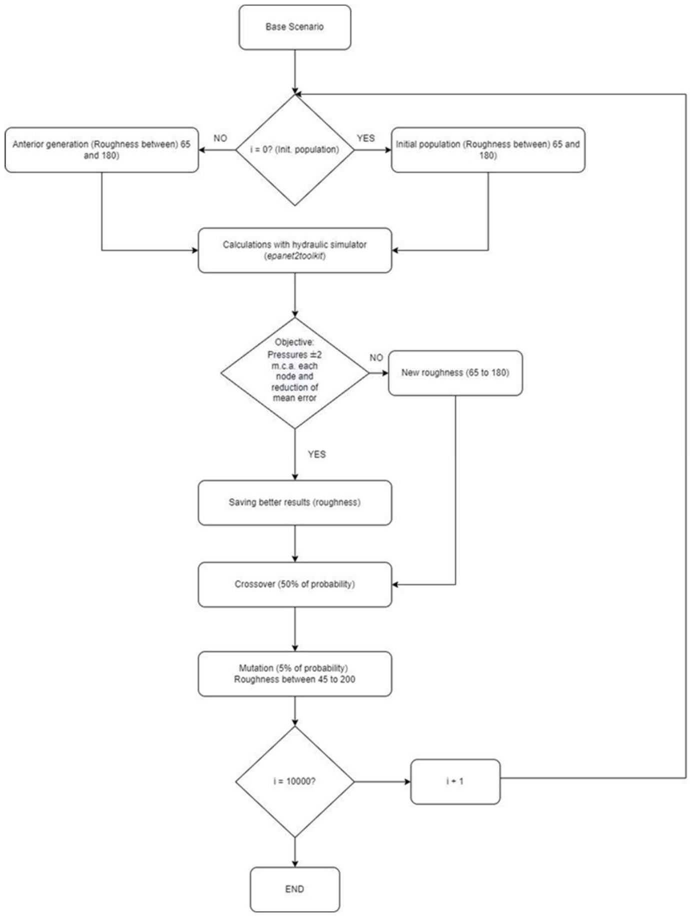

Figure 5: Genetic Algorithm Flowchart

Elaboration of the Genetic Calibration Algorithm

Implementation was done in Python language, but using the same R library, epanet2toolkit. The connection between the two languages took place through the rpy2 package, which allows the use of R libraries and commands in Python. The algorithm has 10,000 generations per simulation, with a 5% chance of mutation and a 50% chance of crossover, as can be seen in the flowchart in Figure 5. Its objective is to perform a calibration with a maximum of ±2 m.c.a. for each individual pressure, not admitting negative pressures and aiming whenever possible to reduce the module of the average of the errors. This algorithm is based on Silva et al. (2022).

Elaboration of Artificial Neural Networks used in calibration

The Artificial Neural Networks used, as in the case of Genetic Algorithms, were also implemented in Python using the rpy2 library to import the R epanet2toolkit library. The input layer consists of the demand data of the network to be calibrated and the output layer consists of the roughness of the pipes, while the hidden layer consists of the input layer plus four neurons, based on Silva et al. (2022). Its operation is explained in the flowchart in Figure 6.

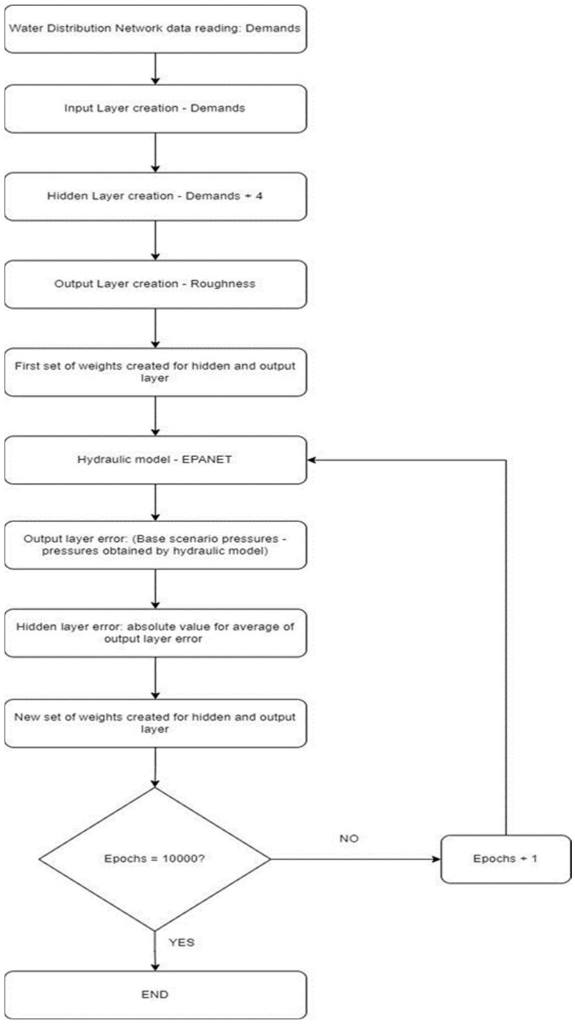

Figure 6: Flowchart of the creation of Artificial Neural Networks

RESULTS

The results of the calibrations for the simple network are shown in Figure 7.

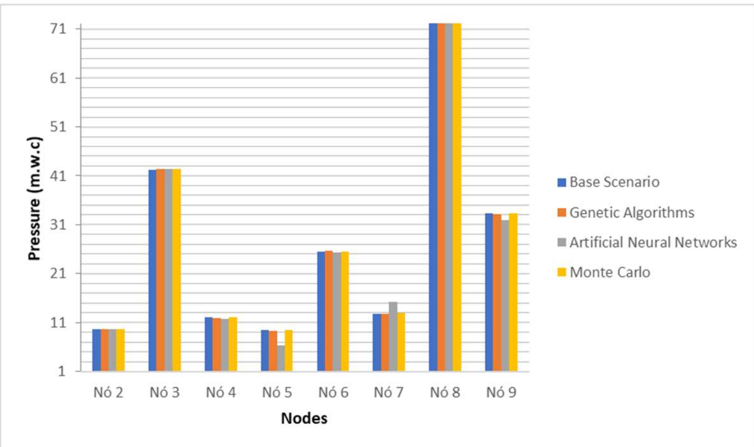

Figure 7: Calibration results for the simple network.

The absolute percentage errors are contained in Table 4, where MC is Monte Carlo, GA is Genetic Algorithms and ANN is Artificial Neural Networks.

Table 4: Percentage error of the algorithms.

Node	Error MC %	Erro GA (%)	Erro ANN(%)
5	0,11%	0,00%	0,31%
6	0,10%	0,07%	0,19%
4	0,41%	0,75%	2,57%
3	0,75%	0,85%	32,48%
9	1,09%	0,82%	0,59%
8	0,86%	0,08%	19,24%
7	0,00%	0,01%	2,85%
2	0,46%	0,48%	3,93%

For the complexe network, the results can be observed in the graph in Figure 8.

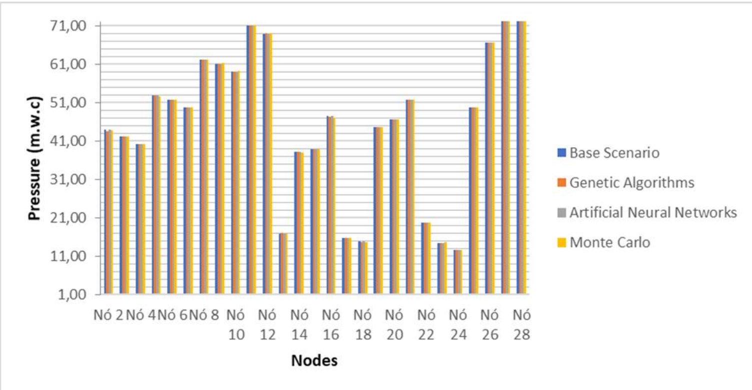

Figure 8: Calibration results for the complex network.

The errors in absolute percentage are contained in Table 5, and due to the performance of the Artificial Neural Networks, five decimal places were adopted after the decimal point for a better expression of the error.

Table 5: Percentage error of the algorithms for the complex network

Node	Error MC %	Erro GA (%)	Erro ANN(%)
2	0,57%	1,03%	0,00000%
3	0,11%	0,21%	0,00924%
4	0,11%	0,22%	0,00007%
5	0,17%	0,02%	0,00829%
6	0,02%	0,07%	0,00290%
7	0,03%	0,04%	0,00330%
8	0,00%	0,08%	0,00696%
9	0,10%	0,02%	0,00206%
10	0,16%	0,08%	0,00753%
11	0,14%	0,06%	0,00722%
12	0,20%	0,09%	0,00657%
13	0,47%	0,67%	0,01442%
14	0,52%	0,11%	0,01255%
15	0,11%	0,14%	0,00734%
16	0,77%	0,25%	0,00019%
17	0,21%	0,51%	0,00824%
18	0,14%	0,41%	0,02583%
20	0,08%	0,12%	0,00977%
21	0,05%	0,02%	0,01000%
22	0,12%	0,01%	0,00866%
23	0,09%	0,07%	0,01577%
24	1,53%	0,40%	0,03410%
25	0,17%	0,17%	0,03651%
26	0,04%	0,10%	0,00428%
27	0,04%	0,10%	0,00703%
28	0,05%	0,10%	0,00113%
29	0,05%	0,10%	0,00111%

DISCUSSION

In the simple network, the best result for the Genetic Algorithm was obtained in the 3285th generation and it obtained the best performance, followed by the Monte Carlo algorithm, whose largest error was 0.21 m.w.c. and 0.28 m.w.c., respectively, fully in accordance with the Water Research Centre (1989) which establishes as performance criteria for calibration models an error of 0.5 m.w.c. for 85% of monitored points, 0.75 m.w.c. for 95% of monitored points or 2.00 m.w.c. for all monitored points, both of which can be considered models with acceptable performance within the mentioned criteria. The Artificial Neural Networks had the worst performance of all, reaching a maximum error of 32.48% in node 3, with a difference of 3.06 m.w.c. and at nodes 8 and 7, with 2.47 m.w.c. and 2.27 m.w.c., respectively, not meeting the criteria established by the Water Research Centre (1989).

In the larger and more complex network, all algorithms met the criteria of the Water Research Centre (1989), with Genetic Algorithms getting the best result in the 7595th generation and again having a slight advantage over Monte Carlo. In this case, the Artificial Neural Networks were able to calibrate the network with great accuracy, and it was even necessary to increase the number of decimal places after the decimal point to five to express its error. However, if on the one hand there was an excellent performance of the Neural Networks in the calibration, on the other hand there is also the risk that the model will have overfitting, that is, an overfitting to a specific situation that could make the model useless for calibration of other water distribution networks.

In Artificial Neural Networks, two problems are recurrent according to Bejani et al. (2021): Overfitting and underfitting. The first is about an over-suitability of the model for a given situation, making it incapable of making more in-depth generalizations, while the second is about the opposite, that is, the inability of the network to learn the relationships between the data.

Based on the results obtained in this work, initially the Neural Networks used were better adapted to larger and more complex networks than to simpler networks, although tests in water distribution networks of different configurations and sizes are necessary to verify their generalization capacity, in especially if there is any tendency towards underfitting in small and simpler networks, as well as if the good results in larger and more complex networks will be repeated.

The results obtained by the Monte Carlo algorithm were lower than those of the Genetic Algorithms, although they were within the calibration criteria established by the Water Research Center (1989). Its main advantage is that it has been written directly in R language, not requiring libraries such as Python's rpy2, which allows for better performance in terms of runtime when compared to Genetic Algorithms or Artificial Neural Networks that need to access the library indirectly.

CONCLUSIONS

This work confirmed that for the calibration of water distribution networks, the Genetic Algorithms developed in the work are an efficient tool and already validated for use, covering from small and simple networks to more complex networks, being, therefore, a reference in the comparison of the performance of other calibration algorithms. In addition to calibration, the use of the rpy2 library also allows the use of other packages available in R, which opens up a range of possibilities in statistical analysis not only related to the calibration of the network, but also related to its optimization and simulation in general.

The Monte Carlo algorithm is also performed as expected by the calibration criteria and can also be used in problems that require the calibration of a water distribution network reliably. In addition, the Monte Carlo algorithm was developed entirely in R language, which makes its application advantageous, as it works faster and smoother, eliminating the need for libraries that access other languages. On the other hand, Genetic Algorithms, which were written in Python language, needed an rpy2 library that allowed using R packages, thus reducing performance.

The Neural Networks used in this work, although they had an excellent result in the most complex calibration, should be observed with some caution due to the apparent overfitting in this situation and a potential underfitting in the simplest situation. However, there is potential for its use in water distribution network problems as long as these conditions are resolved, and the error parameters that generate the weights for the calculations can be adjusted, as well as an insertion of additional hidden layers, alteration of the number of neurons of the hidden layer or even a combination of these solutions.

Another possibility of use for Neural Networks lies in the operation of water supply networks, being able to learn to operate in response to demand variations, even being able to count on the help of Genetic Algorithms or Monte Carlo to obtain optimal operational strategies. that will serve as a basis for your learning.

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