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Article

Developing Machine Learning Models for Optimal Design of Water Distribution Networks Using Graph Theory-Based Features

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Abstract: This study presents an innovative data-driven approach for the optimal design of water distribution networks (WDNs). The methodology comprises five key stages: Generation of 600 synthetic WDNs with diverse properties, optimized to determine optimal component diameters; Extraction of 80 topological and hydraulic features from the optimized WDNs using graph theory; Preprocessing and preparation of the extracted features using established data science methods; Application of six feature selection methods (Variance Threshold, k-best, chi-squared, Light Gradient-Boosting Machine, Permutation, and Extreme Gradient Boosting) to identify the most relevant features for describing optimal diameters; and Integration of the selected features with four machine learning models (Random Forest, Support Vector Machine, Bootstrap Aggregating, and Light Gradient-Boosting Machine), resulting in 24 ensemble models. The Extreme Gradient Boosting-Light Gradient-Boosting Machine (Xg-LGB) model emerged as the optimal choice, achieving R² and RMSE values of 0.98 and 0.02, respectively. When applied to a benchmark WDN, this model demonstrated high accuracy in predicting optimal diameters, with R² and RMSE values of 0.94 and 0.06, respectively. These results underscore the potential of the developed model for accurate and efficient optimal design of WDNs.

Keywords: water distribution networks; graph theory; machine learning; feature engineering; network optimization

1. Introduction

Water distribution networks (WDNs) are complex systems comprising interconnected components such as water supply sources, pipes, and control elements like pumps and valves. These networks play a crucial role in delivering water to consumers at the required pressure and quality. The design of WDNs has garnered significant attention from researchers and designers due to the substantial costs involved (Swamee and Sharma 2008).

The evolution of WDN design approaches has been marked by several key developments. Early efforts in the late 1960s focused on linear programming methods to minimize design costs under hydraulic constraints (Gupta 1969; Karmeli, Gadish, and Meyers 1968; Schaake and Lai 1969). The 1990s saw the rise of nonlinear programming techniques (Su et al. 1987, Duan et al. 1990, and Samani and Naeeni 1996). In recent years, metaheuristic algorithms have gained prominence for their ability to reduce costs effectively (Murphy and Simpson 1992; Savic and Walters 1997; Simpson, Dandy and Murphy 1994). As WDNs have grown more complex, multi-objective optimization algorithms have been developed to address additional factors such as reliability, water quality, and resilience (Creaco

and Franchini 2014; Farmani, Walters and Savic 2005, 2006; Prasad and Park 2004; Riyahi, Bakhshipour and Haghighi 2023; Todini 2000).

Graph theory has emerged as a powerful tool for describing and analyzing WDNs. This approach represents WDNs as a set of nodes (consumers or hydraulic control components) connected by links (pipes) (Bondy and Murty 1976). The application of graph theory to WDNs began in the 1970s, initially focusing on understanding basic concepts and analyzing water flow and pressure (Hamam and Brameller 1971; Kesavan and Chandrashker 1972). Over time, researchers have adopted a more topological perspective, combining graph theory with analytical tools to develop innovative solutions for WDN analysis and design (Riyahi et al. 2024a).

Graph theory has found diverse applications in WDN research, including reliability analysis (Jung et al. 2016), network dimension reduction (Ulanicki et al. 1996; Giudicianni et al. 2019), robustness enhancement (Ostfeld 2005; Yazdani and Jeffrey 2010; Yazdani et al. 2011; Ulusoy et al. 2018), leak detection (Rajeswaran et al. 2018; Di Nardo et al. 2018a), network segmentation (Riyahi et al. 2024b; Tzatchkov et al. 2016; Deuerlein 2008), and pump operation planning (Price and Ostfeld 2016a, 2016b).

The integration of graph theory and machine learning has led to powerful new approaches in WDN analysis and management (Ahmed et al. 2024). This combination enables the extraction of topological features and the identification of complex patterns within WDNs. Applications of this synergy include leak detection and localization (Coelho et al. 2020; Arsene et al. 2012; Kang et al., 2017), water quality monitoring and prediction (Amali et al. 2018), pressure and demand forecasting (Liy-González et al. 2024), sensor and valve placement optimization (Cheng and Li 2023), district metered area design (Di Nardo et al. 2015, Han and Liu 2017), and asset management and failure prediction (Chen and Guikema 2020, Grammatopoulou et al. 2020, Xia et al. 2022).

Unlike traditional methods, which used hydraulic equations to design WDNs and determine the optimal pipe diameter, this study aims to alter the optimal design of WDNs by combining graph theory with machine learning models. The approach involves generating synthetic WDNs, optimizing their design, extracting topological and hydraulic features, and applying machine learning techniques to discover patterns for optimal diameter design. The process includes data preparation, feature selection using six methods, and the creation of 24 ensemble machine learning models. The best-performing model is then applied to the Hanoi WDN, demonstrating the effectiveness of this innovative approach in optimizing WDN design.

2. Methodology

This section introduces an innovative approach to water distribution network (WDN) design using supervised machine learning regression models. The method leverages topological and hydraulic features to achieve optimal WDN design without relying on traditional hydraulic equation-solving techniques. As illustrated in Figure 1, the approach consists of five key steps:

- 1. Generation and optimization of 600 synthetic WDNs to determine optimal pipe diameters.
- 2.Extraction of topological and hydraulic features for WDN components (pipes, nodes, and overall network graph).
 - 3. Preparation of a database using the features obtained in step 2.
 - 4. Application of six feature selection methods to identify the most relevant features.
- 5. Combination of the feature selection methods with four machine learning models, creating 24 ensemble machine learning models to detect optimal WDN design patterns.
- 6.The methodology concludes by applying the most effective ensemble machine learning model to identify optimal diameters for the Hanoi WDN, a real-world case study.

This approach represents a significant departure from traditional WDN design methods, potentially offering improved efficiency in determining optimal pipe diameters. The subsequent sections of the paper will provide detailed explanations of each stage in the proposed methodology.

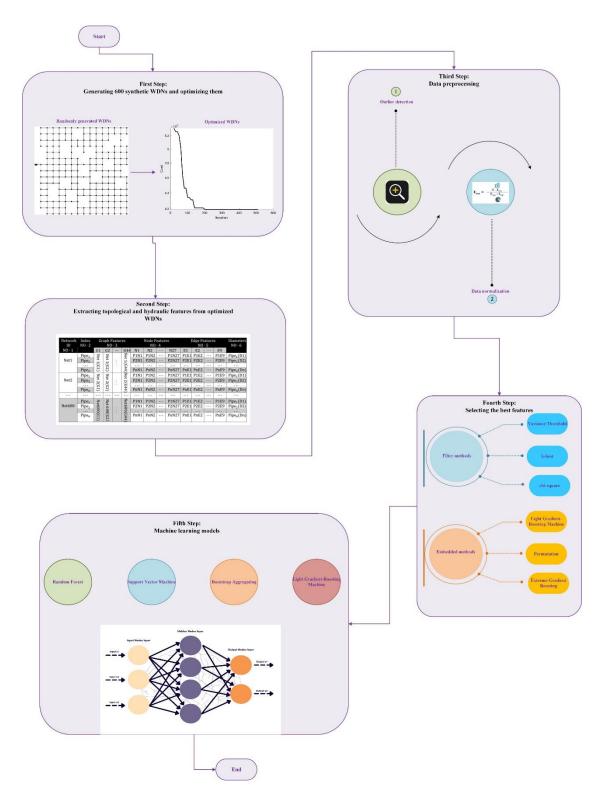


Figure 1. Flowchart of the developed machine learning model based on graph theory for water distribution network design.

2.1. Synthetic Water Distribution Network Generation

Diverse datasets of water distribution networks (WDNs) are essential for simulating and evaluating machine learning and graph theory-based methods. To achieve this, a specialized algorithm was developed to randomly generate WDNs that replicate the characteristics of real-world networks. By adhering to the structural rules that define actual WDNs, the algorithm ensures that the generated networks are both valid and functional. For example, the algorithm produces planar

graphs where all connections (i.e., pipes) are joined exclusively at nodal points. This feature prevents unrealistic pipe connections and closely mirrors the structure of real WDNs.

Additionally, the number of pipes connected to a single node is limited to a maximum of four, further enhancing the resemblance to real networks by avoiding nodes with an excessive number of connections. These constraints, combined with other critical characteristics such as pipe lengths and friction coefficients, help create synthetic WDNs with acceptable similarity to real-world systems.

In this study, 600 synthetic WDNs were generated, with each network component having the following characteristics:

Number of nodes: Between 16 and 141 nodes Number of pipes: Between 24 and 252 pipes Pipe lengths: Between 20 and 100 meters

Hazen-Williams friction coefficient: In the 80 to 130 range

Reservoir head height: Between 20 and 90 meters **Number of loops:** Between 9 and 112 loops

It is also important to note that the elevation of all nodes in these synthetic WDNs was set to zero. By incorporating these features, the generated datasets provide a robust foundation for evaluating machine learning models and graph theory-based approaches in WDN analysis.

2.2. Water Distribution Network Optimization

A primary goal in WDN design is to adequately meet consumer water needs at appropriate pressure levels while also minimizing design costs. A typical approach to achieving such a goal is single-objective optimization, where the objective function is formulated to reduce network construction cost. The main aim of such an optimization is to obtain values of the decision variables (pipe diameters) for which the objective function value (WDN cost) is minimum and the technical and hydraulic constraints within the system are satisfied. The objective function and pressure constraint employed in the optimization problem are presented as follows.

$$f = \sum_{i=1}^{Np} C(d_i) L_i; i = 1, ..., Np (1)$$

$$H_j \ge H_{min};$$
 $j = 1, ..., Nn$ (2)

Equation (1) represents the objective function of the single-objective optimization algorithm. Here, $C(d_i)$ is the cost of diameter d_i per unit of pipe length, and L_i is the pipe length. Equation (2) is the optimization problem constraint, where H_j is the pressure at nodes (j), which must be greater than or equal to the minimum pressure (H_{min}) . The commercial diameters used in optimization problem and their corresponding costs are presented in Table 1. Hydraulic simulation of the randomly generated WDNs is performed in EPANET software (Rossman et al. 2020). To this end, the synthetic graphs created in Python are first introduced to EPANET using the EPANET Toolkit in Python (Kyriakou et al. 2023). Next, specifications for components, such as pipe diameter, pipe length, and nodal consumptions, are assigned to these components, and the hydraulic simulation is performed (Kyriakou et al. 2023). A single-objective genetic algorithm is used in this study to optimize the synthetic WDNs. A self-adaptive method is utilized to satisfy the pressure constraint. Please refer to the article by Makaremi et al. (2017) for further study about the self-adaptive method.

Table 1. Commercial diameters and their corresponding costs.

	1 0
Diameter	Cost of pipes
(mm)	(€)
16	10.34
20	11.18
25	12.22
32	13.69
40	15.36
50	17.45
63	20.17
75	22.67
90	25.81
110	30.89
125	35.38
160	48.84
200	66.80
250	95.25
315	141.83
400	216.60
500	327.50
600	438.40
800	660.20
1000	882.00

2.3. Topological and Hydraulic Features

The integration of topological and hydraulic features significantly enhances the application of machine learning models in water distribution network (WDN) analysis. Topological features, such as node degree, clustering coefficient, and shortest path, define the network structure and connections, offering valuable insights into its inherent organization and stability. Complementing these are hydraulic features that reflect WDN performance, including average flow velocity in pipes, pressure head at nodes, and flow rates under various conditions.

This study incorporates 80 diverse features as critical input variables for various machine learning algorithms. These features enable supervised machine learning models to learn complex

relationships within WDNs, facilitating optimal design without solving hydraulic equations directly. The features used in this research encompass nodes, pipes, and the overall network graph.

Feature assignment follows a specific methodology:

- Node and overall network graph features are assigned to pipes.
- For each pipe, the average of features from connecting nodes is calculated and assigned as a descriptive feature.
- Features derived from the overall network graph are uniformly applied to all pipes within that network, aiding in network differentiation during the learning process.

The study employs both directed and undirected graph representations:

- Undirected graphs are used for features such as square clustering coefficient, node eccentricity, and pipe length index.
- Directed graphs are necessary for features like degree of centrality and shortest path from the reservoir to nodes.
- Some features, including node closeness centrality index and betweenness centrality indices, require examination of both directed and undirected graphs.

Water flow direction determines the graph directionality in WDNs. For features requiring graph weight attributes, either pipe length or the pipe resistance coefficient from the Hazen-Williams equation is used:

$$R = \frac{10.67 \times L_i}{C^{1.85} \times d_i^{4.87}} \tag{3}$$

where:

R = Pipe resistance

 L_i = Pipe length

C = Hazen-Williams coefficient

 d_i = Pipe diameter

The target feature in this study is the optimal commercial diameters in WDNs, obtained through the optimization process. Table 2 presents a schematic of the features derived from 600 artificial networks. For a comprehensive list of features used in this study, please refer to Table A1 in the article Appendix.

Table 2. The features obtained from synthetic WDNs.

Networ k	Inde x		Graph F				Node Fe		es	I	Edge Fe		s	Diamete rs
ID NO.1	NO.	G1	G2		G44	N1	N2		N27	E1	E2		E9	NO.6
	Pipe					P1N 1	P1N 2	•••	P1N2 7	P1E 1	P1E 2	•••	P1E 9	Pipe ₁ (D1
Net 1	Pipe 2	Net 1(C	 Net 1(G2) Net 1(G1)	:	Net 1(G44)	P2N 1	P2N 2	•••	P2N2 7	P2E 1	P2E 2	•••	P2E 9	Pipe ₂ (D2
		1)		44)		•••		•••						
	Pipe					P _n N	P _n N		PnN2 7	PnE 1	PnE 2		PnE 9	Pipen(D n)

	Pipe					P1N	P1N		P1N2	P1E	P1E		P1E	Pipe ₁ (D1
	1					1	2	•••	7	1	2	•••	9)
	Pipe					P2N	P2N		P2N2	P2E	P2E		P2E	Pipe ₂ (D2
Net 2	2	Net 2(G1)	Net 2(G2)	÷	Net 2(G44)	1	2	•••	7	1	2		9)
		31)	32)		44)									
	Pipe					PnN	PnN		PnN2	PnE	PnE		PnE	Pipen(D
	n					1	2	•••	7	1	2	•••	9	n)
	Pipe					P1N	P1N		P1N2	P1E	P1E		P1E	Pipe ₁ (D1
	1					1	2	•••	7	1	2	•••	9)
	Pipe	7	7		Z	P2N	P2N		P2N2	P2E	P2E		P2E	Pipe ₂ (D2
Net 600	2	Net 600(G1)	Net 600(G2)	÷	Net 600(G44)	1	2	•••	7	1	2	•••	9)
		(G1)	(G2)		G44)									
	Pipe					PnN	PnN		PnN2	PnE	PnE		PnE	Pipen(D
	n					1	2	•••	7	1	2		9	n)

2.4. Database Preparation

The critical stage of database preparation follows the development of the algorithm for randomly generating WDNs and extracting their topological and hydraulic features. This process is essential for creating a suitable dataset for machine learning algorithms and involves two key steps:

- Outlier Data Detection: Identifying and handling outliers is crucial as these anomalous values
 can significantly impact model training, reducing accuracy and generalizability. In this study
 outliers are defined as data points that differ by more than four times the standard deviation
 from the mean of the same data set. Once identified, outliers are removed from the final
 database.
- 2. Data Normalization: Normalization is performed using the Min-max normalization method. This step is vital for (1) aligning features with different scales, and (2) preventing disproportionate impact of varying value ranges (e.g., pipe lengths vs. node pressures) on machine learning model performance.

By carefully addressing outliers and normalizing the data, we ensure that the machine learning algorithms have a clean, well-prepared dataset to work with, ultimately leading to more reliable and accurate results in WDN analysis and design.

2.5. Feature Selection Methods

Feature selection is a critical step in machine learning model usage, particularly when dealing with datasets containing a large number of features. This process involves identifying and selecting the most relevant and informative features from the original dataset for training a machine learning model. The primary objectives of feature selection are to enhance model performance, mitigate overfitting, accelerate training, and often provide better model interpretability (Zheng and Casari 2018; Venkatesh and Anuradha 2019).

Feature selection methods can be broadly categorized into four groups: Hybrid, Embedded, Wrapper, and Filter, with each method being suitable for feature extraction in different domains (Chandrashekar and Sahin 2014). The present study employs Filter and Embedded categories. Methods such as Var, Kb, and Chi2 fall under the Filter category, while methods like LGB, Per, and Xg belong to the Embedded group.

In Embedded methods, it is essential to tune the hyperparameters of the machine learning model. The selection of the optimal hyperparameter configuration directly impacts model performance (Yang and Shami 2020; Probst et al. 2018). In this study, the Grid search method is used for hyperparameter tuning, which is a theoretical decision-making approach that involves a comprehensive search for a fixed range of hyperparameter values (Injadat et al. 2020).

In the following the detailed explanations of all six feature selection methods used in this study is given.

1. Chi2

This statistical test is specifically used to examine the dependency between two variables (Liu and Setiono 1995). In feature selection, the chi2 method selects non-negative features that demonstrate the highest statistical dependency on the target variable (Khomytska et al. 2023). In this method, the chi2 value is calculated between each feature and the target variable, with higher chi2 indicating a stronger dependency between the feature and the target. Accordingly, features with larger chi2 values are selected as important features. This method is also well-suited for categorical data, with understanding the concept of variable dependency being relatively straightforward. The main limitation of this method involves its limited applicability to non-negative features and the target variable.

2. Var

In this simple and fast method, features that show little variation, meaning those with low variance, are removed from dataset (Guyon et al. 2003). The central concept is that features that are almost constant tend not to provide valuable information for the machine-learning model (Fida et al. 2021). A variance threshold is determined to apply this method, with features with variances lower than this value removed from the feature set. Due to its simplicity and high speed, this method is often used as a preprocessing stage for data dimension reduction. However, it should be noted that this method only examines features individually and ignores potential interactions between features. Additionally, selecting an appropriate value for the variance threshold can be somewhat arbitrary and data-dependent.

3. Kb

This method aims to select the K most relevant features to the target variable (Desyani et al. 2020). For this purpose, univariate statistical tests evaluate the relationship between each feature and the target variable. The functions used in this method assign a score to each feature based on statistical criteria. Subsequently, the K features that have obtained the highest scores are selected as the optimal features. Furthermore, the chi2 test can also be used as a scoring function for non-negative features. This method is relatively fast and efficient and can sufficiently identify features related to the target. However, much like the variance threshold method, Kb method does not account for the interactions between features. It assumes that the relationship of each feature with the target can be independently evaluated.

4. LGB

LGB is a robust gradient-boosting framework that inherently provides the ability to calculate and deliver feature significance scores (Ye et al. 2019; Hua 2020). This score indicates the impact of each feature on the building of the decision trees in the boosting model. During model training, LGB calculates metrics such as the number of times a feature is used to split nodes in trees, otherwise known as "split," or the reduction in node impurity due to using that feature, otherwise known as "gain." These values are indicators of feature significance. This approach has the advantage of feature selection being directly integrated into the model training process while accounting for the

interactions between features. The key hyperparameters of this method, which are tuned before the training process using Grid search, include n_estimators, num_leaves, max_depth, and learning_rate.

5. Per

This method is applied to evaluate the relative significance of features after training a machine-learning model (Altmann et al., 2010). The model is first employed to predict the significance of any feature. Next, the feature values in the validation set are randomly shuffled. After this alteration, the model's performance on the altered data is evaluated. A significant drop in performance following the randomization of feature values indicates that the feature is of high significance to the model since the disturbance of its values significantly impacts the model's ability to predict. The advantage of this approach is that it can be used for any trained model, and its conceptual basis is relatively easy to understand. However, it can be computationally costly for large datasets with a high number of features, as it would imply re-evaluating the model performance for every feature. As the model employed in this process is LightGBM, hyperparameters from the previous section are employed.

6. Xg

Like LGB, Xg is a popular gradient-boosting algorithm that offers feature significance calculation (Hsieh et al. 2019; Alsahaf et al. 2022). Xg, while training the model, assigns feature importance scores in terms of how often a feature is employed for splitting nodes, the split criterion's contribution from the feature-induced split, and the number of samples that are covered by splits of the feature or "coverage." Similar to LGB feature importance, this approach comes with model training inherently and considers interaction among features. It must be noted that the calculated feature significance is specific to the Xg model and may produce different results for other models. The tuned hyperparameters for the current research study are n_estimators, eta, gamma, and max_depth.

2.6. Machine Learning Models

Machine learning is a branch of artificial intelligence that enables computers to learn from data without explicit programming. In other words, instead of providing computers with step-by-step instructions to perform a task, large volumes of data are provided, with specific algorithms being employed to help the computer identify patterns, relationships, and rules within said data and make predictions or decisions based on this knowledge (Riyahi et al. 2018). The primary goal of machine learning is to develop systems that can improve their performance over time with the reception of additional data. This improvement could involve various areas such as prediction accuracy, processing speed, or the ability to recognize more complex patterns.

2.6.1. Regression in Machine Learning

Regression is one of the most critical and widely used aspects of supervised machine learning. Regression problems aim to establish a relationship between input and output variables. In this context, a relationship is developed to predict a continuous objective variable based on one or more predictor variables (Han et al. 2011). In the present study, four machine learning models, namely RF, SVM, BAG, and LGB are used in regression problems, which will be outlined in detail in the following sections.

1. Random Forest (RF)

The initial idea of the random forest was presented in 1972 by Messenger and Mandell (Messenger and Mandell 1972). This concept was later developed by Cutler et al. (2012). The random forest model is one of the most widely used algorithms in machine learning for classification and regression (Breiman 2001). This model is built on decision trees that are combined to increase prediction accuracy and stability. The main concept here is that each tree is trained independently, and each of said trees makes different decisions regarding the data. The final result is then obtained through voting (for classification problems) or averaging (for regression problems) among the trees. The advantages of random forest include stability and high accuracy. By reducing overfitting and

providing diversity in predictions, this model achieves high accuracy in complex problems. Another advantage of the random forest model is its resistance to noise. Specifically, this model is less sensitive to noise and incorrect data due to the utilization of multiple trees. The adjusted hyperparameters of this method in the present study include n_estimators, min_samples_split, and max_depth.

2. SVM

SVM is one of the powerful and widely used algorithms in supervised machine learning (Cortes and Vapnik 1995). This algorithm is specifically used in classification and regression problems. The main concept behind SVM is locating an optimal hyperplane that separates data in the best possible way. The "optimal hyperplane" denotes locating a hyperplane that maximizes the margin. The margin refers to the distance between the hyperplane and the closest data points from objective function value. These close points are called "support vectors" and play a key role in determining the hyperplane position (Vapnik 2013). In other words, only these points impact the hyperplane location, with other data points having zero impact. SVMhas multiple advantages. This algorithm performs particularly well in high-dimensional spaces and is memory-efficient due to its focus on support vectors. Nevertheless, SVMs are still recognized as valuable tools in the machine learning toolkit due to their high accuracy and decent generalization capabilities. Thus, they are widely used in various fields, including machine vision, natural language processing, and bioinformatics (Scholkopf and Smola 2018; Ben-Hur and Weston 2010). The adjusted hyperparameters of this method in the present study include regularization parameter (C), Kernel, and gamma.

3. BAG

This idea was first used by Breiman et al. (1996) to predict classification and regression models, where they evaluated different models by varying the number of bags, with the results ultimately showing an increase in accuracy through the use of the combined BAG model (Breiman 1996). The BAG model approach is an ensemble learning process that creates multiple instances of a learner, a classifier in this case, to result in multiple predictions (Gaikwad and Thool 2015). The final model output is obtained using a combination rule (i.e., majority voting) of outputs from each created subspace. The generation of multiple samples is conducted by creating self-initiated iterations from the learning set, where samples are randomly drawn from the entire training data with replacement, placing the same number of samples in each subset (Tuysuzoglu and Birant 2020). The adjusted hyperparameters in this method in the present study include n_estimators, max_samples, and max_features.

4. LGB

The initial concept of boosting learning methods was presented by Schapire (1990). In this learning model, the goal is to boost performance. The performance of this method involves implementing a weak learner on the data, which is then enhanced to a strong learner in subsequent stages (Ke et al. 2017). The boosting learning method consists of various types, including the Gradient Boosting model, which transforms a weak learner into a strong learner. The LGB model is an optimized version of the Gradient Boosting framework designed for efficient regression and classification, particularly for high-dimensional data.

The risk of overfitting increased in previous models with increased tree depth, given the Level-Wise logic, which incrementally increased tree depth during training to improve model accuracy. However, in the new logic of the LGB algorithm, the enhancement and training process is Leaf-Wise, meaning that the best branching between leaves (features) is selected in each stage of the decision tree. This process is quite effective in increasing computational speed and reducing overfitting risk. The fundamental hyperparameters of this method were previously described in earlier sections.

2.6.2. Model Evaluation

Two criteria, R^2 and RMSE, are used to evaluate machine learning models. These criteria demonstrate the effectiveness and suitability of machine learning models for the dataset. The R^2 criterion indicates how much of the variance in the objective variable is explained by the model

(Kutner et al. 2004). Furthermore, the RMSE criterion shows how far the predicted values are from the actual values. The relationships between these two criteria are as follows:

$$R^{2} = 1 - \frac{\sum_{i=1}^{n} (y_{i} - \hat{y}_{i})^{2}}{\sum_{i=1}^{n} (y_{i} - \bar{y})^{2}}$$

$$(4)$$

$$RMS = \sqrt{\sum_{i=1}^{n} \frac{(y_i - \hat{y}_i)^2}{n}}$$
 (5)

The values y_i , \hat{y}_i , \bar{y} , and n are outlined below:

- y_i : The real value of the objective variable.
- \hat{y}_i : The predicted value of objective variable.
- \bar{y} : The mean value of objective variable.
- *n*: The total number of samples.

2.6.3. Hanoi WDN

The most effective machine learning model, as determined by the comparative analysis, is selected for application to the Hanoi Water Distribution Network (WDN). Originally introduced by Fujiwara and Khang in 1990, the Hanoi WDN serves as a benchmark case study in water distribution system optimization. This network consists of 32 nodes, 34 pipes, 3 loops and 1 reservoir with a water elevation of 100 meters.

Key hydraulic parameters of the Hanoi WDN include:

- Minimum pressure head at demand nodes: 30 meters
- Hazen-Williams coefficient for all pipes: 130

Figure 2 provides a visual representation of the Hanoi WDN layout, illustrating the network's topological structure and component relationships.

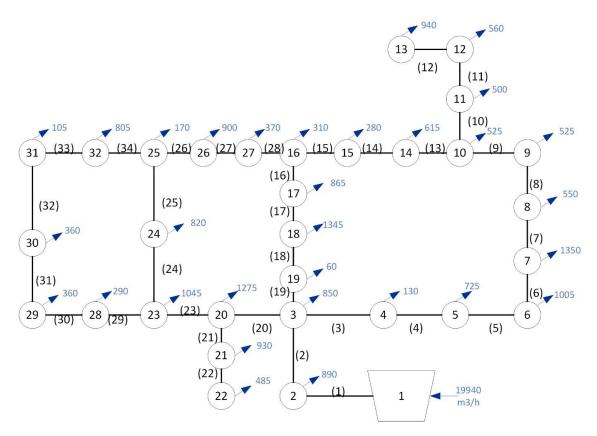


Figure 2. Hanoi WDN.

Figure 2 presents the demand at each node. Additionally, the pipe lengths in order of their respective numbers are: {100, 1350, 900, 1150, 1450, 450, 850, 850, 800, 950, 1200, 3500, 800, 500, 550, 2730, 1750, 800, 400, 2200, 1500, 500, 2650, 1230, 1300, 850, 300, 750, 1500, 2000, 1600, 150, 860, 950}. Five commercial pipe diameters are utilized in the design of the Hanoi WDN: 12, 16, 20, 24, 30, and 40 inches.

3. Results and Discussion

The first stage in the developed model involves the generation of synthetic WDNs. This process utilizes a developed algorithm that includes the graph mining library in Python (NetworkX), the EPANET Toolkit in Python (EPyT), and the genetic algorithm optimizer (geneticalgorithm2). Figure 3 shows the output of three synthetic WDNs. As evident from these WDNs, all components of the generated networks are interconnected, with no pipes interfering with each other. The minimum and maximum number of pipes connected to each node are 1 and 4, respectively. Finally, appropriate random values are assigned to each component of the generated networks to enable the hydraulic design process. For instance, as previously mentioned, pipe lengths are assigned values between 20 and 100 m, or the Hazen-Williams coefficient in pipes is assigned values between 80 and 130. Following the generation of 600 synthetic networks, the design process for the optimal WDN diameters begins. The number of genetic algorithm iterations is 400 iterations on average. Additionally, population size, mutation probability, and crossover probability are set to 12 times the WDN pipes, 0.06, and 0.85, respectively.

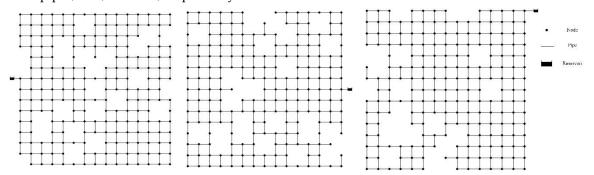


Figure 3. Generated synthetic WDNs.

The topological and hydraulic features are extracted from the WDNs during the next stage. These features generally concern the topological and hydraulic properties of nodes, pipes, and the overall network graph, totaling 80 characteristics, with the target feature being the optimal pipe diameters. The features obtained for nodes are assigned to the pipes connected to them. This assignment is conducted by calculating the arithmetic mean of the features of the nodes at both sides of each pipe and assigning it as the corresponding pipe feature. Regarding the features obtained for the overall network graph, each extracted feature is assigned to all pipes in that WDN. For instance, the network efficiency feature (G7) illustrated in Table 3 is repeated for all pipes in the WDN with the same G7 value. The features extracted at this stage are presented in Table 3. The dataset, which comprises 80 features for 600 synthetic WDNs, has been uploaded to the GitHub site (https://github.com/bahrami-i/WDNs-Dataset), where readers can conveniently download it for use in their research.

Table 3. First and last rows of extracted features from WDNs.

Index		Graph I	Feature	s		Node Fe	eatures			Edge F	eature	es	Diameters
	G1	G2		G44	N1	N2		N27	E1	E3		E9	(mm)
0	379	407		3749	2.50	0.50		11.80	87	31		0.01	200
1	379	407		3749	2.50	1.00		11.90	108	71		0.00	600
2	379	407		3749	3.50	1.50		13.70	112	94	•••	0.04	125
3	379	407		3749	3.00	1.00		11.90	112	22	•••	0.00	500
4	379	407		3749	3.50	1.50		14.20	111	23	•••	0.20	200
5	379	407		3749	2.50	1.00		15.20	114	29	•••	0.22	50
6	379	407	•••	3749	3.00	1.50		18.70	111	21	•••	0.03	160
7	379	407	•••	3749	3.00	1.50		18.90	111	22	•••	0.00	800
8	379	407		3749	2.50	1.50		18.70	96	92		0.00	400
9	379	407		3749	3.50	2.00		18.50	96	78		0.00	315
85735	484	507		3672	3.00	0.50		28.80	120	46		0.00	250
85736	484	507		3672	3.00	1.50		36.50	118	54		0.30	40
85737	484	507		3672	3.00	1.50		45.00	106	63		0.03	250
85738	484	507		3672	3.00	1.00		46.30	87	38		0.02	315
85739	484	507		3672	3.00	1.50		52.20	88	49		0.22	90
85740	484	507		3672	3.00	1.50		58.80	91	40		0.06	315
85741	484	507		3672	3.00	1.50		63.80	92	89		0.08	315
85742	484	507		3672	3.00	2.00		68.20	83	45		0.03	1000
85743	484	507		3672	3.00	2.00		70.20	90	35	•••	0.01	800
85744	484	507		3672	2.00	1.50		35.80	89	63		0.09	800

The features depicted in Table 3 correspond to 600 synthetic WDNs, with the number of rows equal to 85,745 samples, the same as the number of pipes in 600 artificial networks. There are 80 columns corresponding to the number of features. Following obtaining topographical and hydraulic features, outliers are identified and removed from the dataset. To this end, all characteristics are examined, and the values exceeding 4 times the standard deviation relative to the data mean according to the Z-Score criterion are identified. The rows containing said features are removed from

the dataset. Following the outlier removal process, the number of rows in the dataset decreases from 85,745 to 67,226 rows. Figure 4 compares the frequency histogram of the N4 feature before and after outlier removal. As illustrated, removing outliers has led to variations within the range of the N4 feature.

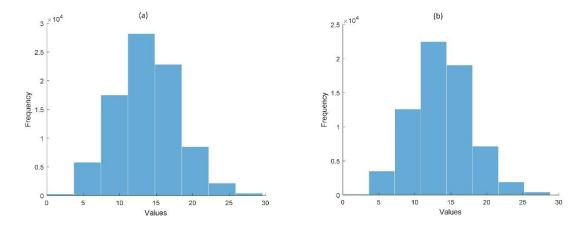


Figure 4. Histogram of the N4 feature before (a) and after (b) outlier removal.

The dataset is then normalized using the min-max normalization method to scale the features within the 0 to 1 range. This data normalization improves machine learning model performance, increases convergence speed in gradient-based algorithms, and prevents characteristics with larger scales from dominating. Table 4 presents the output of Table 3 features following outlier removal and data normalization.

Table 4. First and last rows of extracted features following outlier removal and normalization.

								•	,				
Index	(Graph F	eature	s		Node F	eature	5		Edge Fe	atures		Diameters
	G1	G2		G44	N1	N2		N27	E1	Е3		E9	(mm)
0	0.23	0.04		0.41	0.25	0.00		0.13	0.17	0.14		0.01	0.19
1	0.23	0.04		0.41	0.25	0.20		0.14	0.70	0.64		0.00	0.59
2	0.23	0.04		0.41	0.75	0.40		0.16	0.80	0.92		0.07	0.11
3	0.23	0.04		0.41	0.50	0.20		0.14	0.80	0.02		0.00	0.49
4	0.23	0.04		0.41	0.75	0.40		0.16	0.77	0.04		0.38	0.19
5	0.23	0.04		0.41	0.25	0.20		0.17	0.85	0.11		0.44	0.03
6	0.23	0.04		0.41	0.50	0.40		0.22	0.77	0.01		0.06	0.15
7	0.23	0.04		0.41	0.50	0.40		0.22	0.77	0.02		0.00	0.80
8	0.23	0.04		0.41	0.25	0.40		0.22	0.40	0.90		0.01	0.39
9	0.23	0.04		0.41	0.75	0.60		0.21	0.40	0.73		0.00	0.30

85736	0.55	0.05	 0.39	0.50	0.40		0.42	0.95	0.42		0.56	0.02
85737	0.55	0.05	 0.39	0.50	0.40		0.52	0.65	0.54		0.06	0.24
85738	0.55	0.05	 0.39	0.50	0.20	•••	0.54	0.17	0.22		0.04	0.30
85739	0.55	0.05	 0.39	0.50	0.40		0.61	0.20	0.36		0.44	0.07
85740	0.55	0.05	 0.39	0.50	0.40		0.68	0.27	0.25		0.12	0.30
85741	0.55	0.05	 0.39	0.50	0.40		0.74	0.30	0.86		0.17	0.30
85743	0.55	0.05	 0.39	0.50	0.60	•••	0.82	0.25	0.19	•••	0.15	0.80
85744	0.55	0.05	 0.39	0.00	0.40	•••	0.41	0.22	0.54		0.17	0.80

A visual comparison of Tables 3 and 4 reveals that the row corresponding to index 85,742 in Table 3 has been removed from Table 4, which as previously explained, occurred due to outlier removal. Additionally, it is clear from Table 4 that the data have been normalized between 0 and 1 after data normalization process. The dataset is divided into training and test data sets during the next stage. Seventy percent of the total data is assigned to training data, while thirty percent is designated for test data.

The next stage involves performing essential feature extraction from the 80 existing features in the dataset. To this end, as previously stated, six models, namely Var, Kb, Chi2, LGB, Per, and Xg, are utilized. The Var, Chi2, and Kb models belong to the Filter model category, while the LGB, Xg, and Per models belong to the Embedded category. The hyperparameter tuning in Embedded models is carried out using the Grid search algorithm. Table 5 depicts the hyperparameter values of the Embedded models tuned using the Grid search algorithm. Additionally, Table 6 illustrates the top 20 features provided by the feature selection methods.

Table 5. Hyperparameter Values of Embedded Methods.

Hyperparame	Em	bedded Meth	nods
ter Tuning with Grid search	Xg	LGB	Per
n-estimators	1350	1500	1500
eta	0.250	-	-
gamma	0.002	-	-
Max-depth	15	12	12
Num-leaves	-	45	45
Learning-rate	-	0.011	0.011

 $\textbf{Table 6.} \ \textbf{Selection of top 20 features based on feature selection methods}.$

Methods	Kb	Chi2	Var	LGB	Per	Xg
_	N5	N5	E1	E9	N5	E9
_	N7	N7	E3	E8	N7	N5
_	E5	E5	G43	N5	E3	E8
_	N8	N8	G44	N7	E9	N7
	E9	N17	G7	E3	E1	E1
	E3	E9	G20	E1	E5	E3
	E1	N15	G21	N8	E8	N8
	G42	N19	G23	E5	N8	N10
	N23	E8	G30	N10	N10	E5
Selected Features	G12	N18	G31	N6	N6	N6
	G8	N2	G32	N4	N3	N26
	G4	N10	G35	N17	N17	N4
	G17	N3	G36	N26	N1	E6
	G13	N13	G39	E4	N23	E7
	G10	N6	G41	N19	N25	N17
	G41	E3	N1	N9	N4	N20
	G6	N4	N2	E6	G25	N15
	G18	N14	N5	N18	G3	E4
	G27	N22	N7	E7	G2	N9
	G2	E1	N23	N20	G10	N19
Node features percentage	20	75	25	60	55	60
Pipe features percentage	20	25	10	40	25	40
Over all graph features percentage	60	0.0	65	0.0	20	0.0

The analysis of results feature selection methods in Table 6 reveals several key insights:

Feature importance by category:

- Node-related features dominate in four methods (Xg, Per, LGB, and Chi2)
- Overall network graph properties are most prominent in two methods (Kb and Var) Significance of specific features:
- N5 and N7 (weighted node centrality degrees) consistently appear in the top quartile for most methods, except Var
- Features using pipe resistance (R) as a weighted criterion show greater importance than those using pipe length

Distribution of top features:

- Node features: 50% on average
- Pipe features: 26% on average
- Graph features: 24% on average
 - Method-specific observations:
- Filter methods (e.g., Kb and Var) tend to select more overall network graph features
- Embedded methods (e.g., Xg, Per, LGB) primarily select node and pipe features Application to machine learning:
- Top features from each selection method are paired with corresponding optimal diameters
- These feature sets are used as inputs for four machine learning models
- Hyperparameters for each model are optimized using the Grid search algorithm (detailed in Table 7)

Table 7. Hyperparameter values of machine learning models.

Hyperparameter		Ensemb	le model	
tuning with Grid search	RF	SVM	BAG	LGB
n-estimators	250	-	140	1500
Max-depth	30	-	-	-
Min-samples-split	10	-	-	12
Max-samples	-	-	0.7000	-
Max-features	-	-	0.7500	-
С	-	1.0000	-	-
kernel	-	ʻrbfʻ	-	-
gamma	-	-	0.0001	-
Num-leaves	-	-	-	45
Learning-rate	-	-	-	0.0110

Thus, 24 combined machine learning models are trained and ultimately evaluated with test data. The evaluation metrics used are R^2 and RMSE. Figure 5 shows the output of 24 coupled machine learning models. As observed in this figure, the strongest model based on both evaluation metrics is

the Xg-LGB model, which implements the best features of the Xg method on the LGB regressor, with R^2 and RMSE values at 0.98 and 0.02, respectively. The weakest model is Var-SVM, with R^2 and RMSE values at 0.41 and 0.21, respectively.

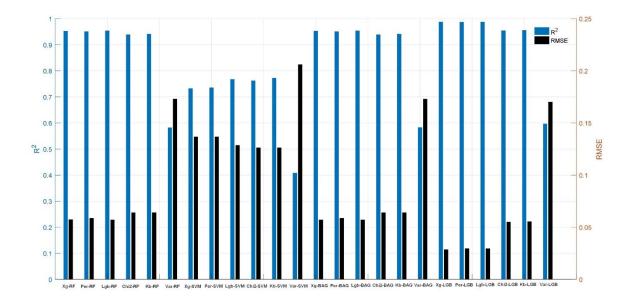


Figure 5. The output of 24 coupled machine learning models.

After selecting the best machine learning method, the Xg-LGB model, this model is used to find the optimal diameters in the Hanoi WDN. The results show that R^2 is 0.94, indicating a high percentage of variance in the objective values (optimal diameters presented by Kadu et al. 2008) identified by the Xg-LGB model. Furthermore, the RMSE value is 0.06, indicating that a small percentage of variance in the objective values remains unidentified by the model due to various factors: a shortage of features, measurement errors, incidental noise, model limitations, and data limitations. By improving each of the mentioned factors, the model's efficiency could be enhanced. Table 8 presents the diameters calculated by the Xg-LGB model for the Hanoi WDN, along with the diameters of this network presented by Kadu. From the table, the diameters obtained by the Xg-LGB model are continuous values and rounded to the nearest commercial diameter. By comparing these diameters with Kadu's findings, it becomes clear that in approximately 65% of cases, the forecasted diameters of the Xg-LGB model are equal to Kadu's outputs, while in the remaining 35%, these diameters are one size larger than Kadu's results. Since Kadu's findings are obtained by applying the genetic optimization algorithm, the high level of consistency in the results predicted by the Xg-LGB model can be reasoned as follows: first, the original synthetic database presented in Table 3 is suitable for generating the optimal diameters for a given number of random WDNs; second, the Xg feature selection method in Table 6 has effectively identified the efficient features corresponding to the objective function; and third, the Xg-LGB model has well been trained concerning the original synthetic database and then to the Hanoi benchmark network, all of which can somehow embody the appropriate generalization of the model.

Additionally, using the predicted diameter results from the Xg-LGB model on the Hanoi WDN and conducting the hydraulic simulation with Epanet software, the nodal pressure heads are obtained, displayed in the last column of Table 8. Except for node 2, which has a pressure of 97.14 meters (due to its proximity to the reservoir), the pressures at other nodes range from 35 to 65 meters. This improves the minimum pressure derived from Kadu's diameter results and meets the maximum pressure requirements, which are essential for ensuring adequate pressure in consumer nodes.

Table 8. The pipe diameters from Kadu and Xg-LGB models and pressure head in each node of Hanoi WDN.

Pipe	\mathbf{P}_{1}	redicted diameters		Node	Pressure head from Xg-LGB model
number	Pipe diameters	Continuous	Commercial	number	(m)
	from Kadu et al.	pipe diameters	pipe diameters		
	(2008)	from Xg-LGB	from Xg-LGB		
	(in)	model	model		
		(in)	(in)		
1	40	38.9	40	1	100.0
2	40	36.9	40	2	97.1
3	40	40.7	40	3	61.6
4	40	40.3	40	4	57.3
5	40	39.9	40	5	52.0
6	40	39.5	40	6	46.5
7	40	39.1	40	7	45.2
8	40	40.0	40	8	43.8
9	30	33.7	30	9	42.6
10	30	35.4	40	10	39.4
11	30	34.9	30	11	39.0
12	24	27.4	30	12	37.
13	16	18.2	20	13	36.
14	12	14.0	16	14	37.8
15	12	13.0	12	15	37.0
16	16	18.4	20	16	38.
17	20	22.1	24	17	45.
18	24	24.4	24	18	51.
19	24	28.2	30	19	60.
20	40	40.0	40	20	51.
21	20	23.4	24	21	47.
22	12	13.1	12	22	42.4
23	40	39.2	40	23	45.9
24	30	34.6	30	24	41.4
25	30	34.4	30	25	38.
26	20	21.4	20	26	36.
27	12	14.1	16	27	36.
28	12	14.6	16	28	39.
29	16	17.6	16	29	36.
30	12	14.5	16	30	36.
31	12	13.0	12	31	36.
32	16	17.6	16	32	36.
33	20	23.9	24		
34	24	26.8	24		

4. Conclusion

The optimal design of WDNs is one of the most critical engineering challenges, directly impacting service quality, economic costs, and water resource sustainability. Given urban population growth and increasing water demand, there is an increasingly urgent need for efficient methods to design these networks. Traditional WDN design methods are often time-consuming and have significant limitations when facing complex networks. Thus, developing novel and intelligent methods that can perform optimal design with high speed and accuracy seems essential.

A novel machine learning-based approach for optimal water distribution network design was presented in this study. To this end, 600 synthetic WDNs were generated and optimized. Then, 80 topological and hydraulic features concerning nodes, pipes, and the overall network graph were extracted from the optimized WDNs. Following data preprocessing, including outlier detection and normalization, six feature selection methods, namely Chi2, Var, Kb, LGB, Permutation, and Xg, were employed. Subsequently, four machine learning algorithms, including RF, SVM, LGB, and BAG, were utilized in combination with feature selection methods. Results showed that the LGB-Xg method had the best performance based on R^2 and RMSE in optimal WDN design. This combination method not only demonstrated higher accuracy compared to other methods but also showed significant capability in generalizability and predicting optimal pipe diameters. Finally, the LGB-Xg method is applied to a real-world WDN, the Hanoi WDN, demonstrating that this model can predict the optimal pipe diameters with R² and RMSE values of 0.94 and 0.06, respectively. The research results indicated that among node, pipe, and overall network graph features, topological and hydraulic node features are of very high importance. This study demonstrates that using machine learning approaches can significantly improve water WDN design processes. Moreover, the study results can serve as a guideline for engineers and designers in the selection of appropriate pipe diameters in WDNs.

It is recommended that future studies investigate and explore the feasibility of using graph neural networks as an alternative to coupled machine learning models. Additionally, other factors such as reliability and uncertainty could be considered when developing machine learning methods for designing WDNs that achieve optimal diameters and enhance reliability.

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Appendix A

Table A1. Complete List of Features Used in this Study.

	Index		Features Name
	<i>N</i> 1	$Node_{DC}$	Node Centrality Degree
	N2	$Node_{D-Out}$	Output Degree of Directed Graph Nodes
	N3	$Node_{D-In}$	Input Degree of Directed Graph Nodes
Topological	N4	$Node_{DC-InL}$	Internal Weighted Centrality Degree for Weighted
		Trouc _{DC} -InL	Multiplication of Input Edge Lengths by Input
Features			Degree in the Directed Graph
	N5	$Node_{\scriptscriptstyle DC-InRHW}$	Internal Weighted Centrality Degree for Weighted
	143	Noue DC-InRHW	Multiplication of Resistance Index (R) of Input
			Edges by Input Degree in the Directed Graph

Node Features

N6	$Node_{DC-OutL}$	External Weighted Centrality Degree for Weighted Multiplication of Input Edge Lengths by Input Degree in the Directed Graph
N7	$Node_{DC-OutR}$	External Weighted Centrality Degree for Weighted
14 /	Noue _{DC} -outR	Multiplication of Resistance Index (R) of Input
		Edges by Input Degree in the Directed Graph
<i>N</i> 8	$Node_{Ave.Dim}$	Average Diameter of Tubes Connected to Node
N9	$Node_{\mathit{Min.Path.Length}}$	Minimum Weighted Length Distance from
	g	Reservoir to Node in the Directed Graph
N10	$Node_{\mathit{Min.Path.RHW}}$	Minimum Weighted Resistance Distance from
	HULL UULKIIV	Reservoir to Node in the Directed Graph
<i>N</i> 11	$Node_{SCC}$	Node Clustering Coefficient in the Undirected
		Graph
<i>N</i> 12	$Node_{\mathit{CC-Undir-L}}$	Weighted Length Closeness Centrality Index in the
	cc-onan-E	Undirected Graph
N13	$Node_{\mathit{CC-Undir-R}}$	Weighted Resistance Closeness Centrality Index in
	cc-onan-k	the Undirected Graph
N14	$Node_{\mathit{CC-dir-L}}$	Weighted Length Closeness Centrality Index in the
		Directed Graph
<i>N</i> 15	$Node_{\mathit{CC-dir-R}}$	Weighted Resistance Closeness Centrality Index in
		the Directed Graph
N16	$Node_{BC-Undir-L}$	Weighted Length Betweenness Centrality Index in
	BC-Onan-E	the Undirected Graph
N17	$Node_{BC-Undir-R}$	Weighted Resistance Betweenness Centrality Index
	BC-onun-R	in the Undirected Graph
N18	$Node_{BC-dir-L}$	Weighted Length Betweenness Centrality Index in
	вс-ин-Е	the Directed Graph
N19	$Node_{BC-dir-R}$	Weighted Resistance Betweenness Centrality Index
		in the Directed Graph
N20	$Node_{EC-Undir-L}$	Weighted Length Eigenvector Centrality Index in
	EC-Onun-E	the Undirected Graph
<i>N</i> 21	$Node_{EC-dir-L}$	Weighted Length Eigenvector Centrality Index in
	Le un L	the Directed Graph
N22	$Node_{EC-dir-R}$	Weighted Resistance Eigenvector Centrality Index
1422	Nouvec-dir-R	in the Directed Graph
	,	Subgraph Centrality Index in the Undirected
N23	$Node_{SC-Undir}$	Graph
		·
N24	$Node_{{\it EcC-Undir-L}}$	Weighted Length Node Eccentricity Index in the
		Undirected Graph

		N25	$Node_{\it EcC-Undir-R}$	Weighted Resistance Node Eccentricity Index in the Undirected Graph
	Hydraulic	N26	$Node_{Demand}$	Consumption Flow Rates at Nodes
	Features	N27	$Node_{Pressure}$	Pressure at Nodes
Edge	Topological	<i>E</i> 1	$Edge_{Friction}$	Pipe Roughness Index
Features	Features .	E2	$Edge_{Diameter}$	Pipe Diameter Index
		E3	$Edge_{Length}$	Pipe Length Index
		E4	$Edge_{BC-Undir-L}$	Weighted Length Edge Betweenness Centrality
		E5	$Edge_{BC-Undir-R}$	Index in the Undirected Graph Weighted Resistance Edge Betweenness Centrality
				Index in the Undirected Graph Weighted Length Edge Betweenness Centrality
		E6	$Edge_{{\scriptscriptstyle BC-dir-L}}$	Index in the Directed Graph
		E7	$Edge_{{\scriptscriptstyle BC-dir-R}}$	Weighted Resistance Edge Betweenness Centrality Index in the Directed Graph
		E8	$Edge_{Velocity}$	Flow Velocity Index in Pipe
	Hydraulic Features	E9	$Edge_{HeadLoss}$	Energy Loss Index per Pipe Length
	1 00000 05	<i>G</i> 1	Graph _{Ave.Min.Path.L}	Average Minimum Weighted Length Distance from Reservoir to Node in the Overall Directed
		G2	Graph _{Ave.Min.Path.R}	Graph Average Minimum Weighted Resistance Distance from Reservoir to Node in the Overall Directed Graph
		<i>G</i> 3	$Graph_{Dia-Undir-L}$	Graph Diameter of Weighted Length Type in Overall Undirected Graph
		<i>G</i> 4	$\mathit{Graph}_{\mathit{Dia-Undir-R}}$	Graph Diameter of Weighted Resistance Type in the Overall Undirected Graph
		<i>G</i> 5	$Graph_{Rad-Undir-L}$	Graph Radius of Weighted Length Type in the Overall Undirected Graph
		<i>G</i> 6	$Graph_{Rad-Undir-R}$	Graph Radius of Weighted Resistance Type in the Overall Undirected Graph
	•	<i>G</i> 7	$\mathit{Graph}_{\mathit{Effi-Undir}}$	Graph Efficiency in the Overall Undirected Graph
		G8	$Graph_{Ave.CC-Undir-L}$	Average Closeness Centrality Index of Weighted Length Type in the Overall Undirected Graph
		<i>G</i> 9	Graph _{Ave.CC} -Undir-R	Average Closeness Centrality Index of Weighted Resistance Type in the Overall Undirected Graph
		G10	$0 \qquad \qquad \textit{Graph}_{\textit{Ave.CC-dir-L}}$	Average Closeness Centrality Index of Weighted Length Type in the Overall Directed Graph

	Topological Features	G11	$\mathit{Graph}_{\mathit{Ave.CC-dir-R}}$	Average Closeness Centrality Index of Weighted Resistance Type in the Overall Directed Graph
		G12	$Graph_{Ave.BC-Undir-L}$	Average Betweenness Centrality Index of Weighted Length Type in the Overall Undirected
				Graph
	-	G13	$Graph_{Ave.BC-Undir-R}$	Average Betweenness Centrality Index of
Graph				Weighted Resistance Type in the Overall
Features		G14	Graph _{Ave.BC-dir-L}	Undirected Graph
				Average Betweenness Centrality Index of
				Weighted Length Type in the Overall Directed
				Graph
		G15	Graph _{Ave.BC-dir-R}	Average Betweenness Centrality Index of
				Weighted Resistance Type in the Overall Directed
				Graph
		C16	$Graph_{CD-Undir-L}$	Dominance of Central Point of Weighted Length
		G16		Type in the Overall Undirected Graph
		C17	$Graph_{CD-Undir-R}$	Dominance of Central Point of Weighted
		G17		Resistance Type in the Overall Undirected Graph
		610	$Graph_{CD-dir-L}$	Dominance of Central Point of Weighted Length
		G18		Type in Overall Directed Graph
		G19	$Graph_{CD-dir-R}$	Dominance of Central Point of Weighted
				Resistance Type in the Overall Directed Graph
		G20	$Graph_{Ave.Deg-Undir}$	Average Graph Degree in the Overall Undirected
				Graph
		G21	$Graph_{Ave.OutDeg-dir}$	Average Output Degree in the Overall Directed
				Graph
		G22	$Graph_{ ext{Max.Deg-Undir}}$	Maximum Degree in the Overall Undirected
				Graph
		G23	$Graph_{Max.InDeg-dir}$	Maximum Input Degree in the Overall Directed
				Graph
		G24	$Graph_{{ m Max.}OutDeg-dir}$	Maximum Output Degree in the Overall Directed
				Graph
		G25	$\mathit{Graph}_{Ave.\mathit{LCC}}$	Average Node Square Clustering Coefficient in the
				Overall Undirected Graph
		G26	$Graph_{\mathrm{FV-}Undir}$	-
				Algebraic Connectivity Index in the Overall
		G27	Cmank	Undirected Graph
		G2/	$Graph_{FV-Undir-L}$	Algebraic Connectivity Index of Weighted Length
		620	Curul	Type in the Overall Undirected Graph
		G28	$Graph_{\mathrm{FV-}Undir-R}$	Algebraic Connectivity Index of Weighted
		600	C. 1	Resistance Type in the Overall Undirected Graph
		G29	$Graph_{\mathrm{SD-}Undir}$	Spectral Difference of the Overall Undirected
	-			Graph

Hydraulic

Features

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	G30	Graph_{SD-dir}	Number of Edges in the Overall Undirected Graph
_	G31	$Graph_{ m Density-Undir}$	Density of the Overall Undirected Graph
_	G32	$Graph_{ m Density-dir}$	Density of the Overall Directed Graph
-	G33	$Graph_{\mathrm{Mesh-Undir}}$	Mesh Coefficient of Overall Undirected Graph
=	G34	$\mathit{Graph}_{DeadEnd-dir}$	Sum of Input Degrees of Dead-End Nodes in the Overall Directed Graph
=	<i>G</i> 35	$Graph_{NC-Undir-Res}$	Normalized Minimum Cut between Reservoir and First Node with Other Nodes in the Overall Undirected Graph
	<i>G</i> 36	$Graph_{ ext{NC-Undir-Res-}L}$	Normalized Minimum Cut of Weighted Length Type between Reservoir and First Node with Other Nodes in the Overall Undirected Graph
_	<i>G</i> 37	Graph _{NC-Undir-Res-R}	Normalized Minimum Cut of Weighted Resistance Type between Reservoir and First Node with Other Nodes in Overall Undirected Graph
_	<i>G</i> 38	$Graph_{ m NC-Undir-End}$	Normalized Minimum Cut between Terminal Node and Other Nodes in the Overall Undirected Graph
_	G39	$Graph_{ ext{NC-Undir-End-}L}$	Normalized Minimum Cut of Weighted Length Type between Terminal Node and Other Nodes in the Overall Undirected Graph
_	G40	$Graph_{ ext{NC-Undir-End-}R}$	Normalized Minimum Cut of Weighted Resistance Type between Terminal Node and Other Nodes in the Overall Undirected Graph
-	G41	$Graph_{Total \mathrm{Length}}$	Total Network Length in the Overall Graph
_	G42	$\mathit{Graph}_{R_{HW}}$	Overall Network Resistance Index in the Overall Undirected Graph
	G43	$Graph_{ResElv}$	Water Level in Reservoir in the Overall Graph
-	G44	$\mathit{Graph}_{\mathit{TotalDemand}}$	Total Input Flow to Network in the Overall Graph

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