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A Performance Comparison of Unsupervised Machine Learning Algorithms for Clustering Water Depth Datasets at Urban Drainage Systems

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Highlights

1. Noise-free and -polluted water depth datasets of urban drainage systems are used for clustering analysis.

2. The dendrogram cut-off point dominates the number of clusters in agglomerative clustering.

3. The number of clusters is found to be highly-related to sample length but is slightly relevant to data magnitude.

4. Performance of K-means, Agglomerative, and Spectral clustering is assessed by three metrics in grouping time-series water depth datasets.

Abstract As sensor measurements emerge in urban water systems, data-driven unsupervised machine learning algorithms have been drawn tremendous interest in infrastructure monitoring, flow prediction, and pollutant warning recently. However, most of them are applied in water distribution systems, and few studies consider using unsupervised clustering analysis to group the time-series hydraulic-hydrologic data at urban drainage systems. To improve the understanding of how clustering analysis contributes to detecting urban flooding events, this study compared the performance of K-means Clustering, Agglomerative Clustering, and Spectral Clustering in uncovering time-series water depth similarity and finally identified the number of clusters with maximum performance scores. In this work, the water depth datasets are simulated by a real-world SWMM model and then formatted for a clustering problem. Three standard performance evaluation scores, the SCI, CHI, and DBI, are employed to assess the clustering performance under six artificial rainfalls and two recorded storms. The results indicate that SCI and DBI are appropriate for assessing the performance of K-means Clustering and Agglomerative Clustering, while CHI only works for Spectral Clustering. Noticeably, it was found that the number of clusters is negatively related to the dataset length, but less correlated with the dataset magnitude.

Keywords: SWMM modeling, Unsupervised Machine Learning, Clustering analysis, Cluster number, Data features

1. Introduction

Urban drainage systems (UDSs) are the infrastructures constructed to provide conveyance ability and storage capability for surface inundation reduction, drainage overflow mitigation, and pollutant removal. However, the existing UDSs, whose functionality can only serve for a limited number of years, might degrade and even deteriorate as time goes by (Li *et al.* 2019). In recent years, retrofitting the traditional UDSs with water-level sensors, velocity meters, and flow sensors have been widely adopted as an adaptive and cost-effective solution for stormwater challenges (Kerkez *et al.* 2016; Li *et al.* 2019). The deployed sensors can measure the water quantity and quality data in a real-time way, which now makes it feasible for researchers and engineers to tap into the UDSs. The need to understand the emerging data is crucial for forecasting extreme storms, reducing sewer overflows, and predicting flash floods (Morales *et al.* 2017; Norbiato *et al.* 2008; Wong & Kerkez 2016). Interpreting big water data into flood forecasting is attracting increasing attention from researchers (Solomatine & Ostfeld, 2008; Henonin *et al.* 2013; Koo *et al.* 2015; Vojinovic & Abbott 2017; Li *et al.* 2020).

In the last decade, many scholars have introduced a number of machine learning techniques to investigate the available water resources and hydrological datasets (Diao *et al.* 2014; Hsu *et al.* 2013; Kang *et al.* 2013; Mullapudi & Kerkez 2018; Wang *et al.* 2009). Bowes *et al*. (2019) compared long short-term memory and recurrent neural network by using a time-series of groundwater table data in the city of Norfolk, Virginia. They explained that long short-term memory is better than the recurrent neural network in predicting groundwater level, but takes about three times longer to train the model. Hu *et al.* (2018) applied a boosted decision regression tree to forecast flow with over 90% accuracy in combined sewer systems of Detroit city, Michigan. Zhou *et al.* (2019) proposed an accurate deep learning algorithm to locate the pipe burst in water distribution networks by using only 15 or 30 minutes of time-series pressure datasets collection. However, the majority of these studies have focused on supervised learning (i.e., when a known outcome is used to train the model), and unsupervised machine learning algorithms (UMLA) are not commonly used in urban drainage systems.

Clustering analysis, one of the key unsupervised machine learning methods, has been applied in many fields, including pattern recognition, image analysis, data compression, and anomaly detection (Jain *et al.* 1999; Tan *et al.* 2005). In general, cluster analysis is based on identifying similarities between observations. If a water quantity or quality event happens in the water system, these observations are likely to be highly dissimilar to other observations (Wu *et al.* 2016). The increase in dissimilarity would lead to these observations being considered as outliers, and thus detected as anomalies. Although clustering analysis has been extensively discussed in municipal topology classification and water distribution network simplification (Perelman & Ostfeld, 2012, 2011; Sela Perelman *et al.* 2015), the ability of UMLA methods to group time-series data at UDSs is still unknown, and the most appropriate methods to assess these algorithms are unclear. Keogh *et al.* (2003) concluded that clustering time-series data is meaningless, but this argument does not cover the similarity-based clustering algorithms such as K-means and agglomerative clustering. In contrast, Chen (2007, 2005) demonstrated that similarity-based cluster analysis could be successfully applied to sequence datasets by using different distance measures. Wu *et al.* (2016) adopted the clustering algorithm, developed by Rodriguez & Laio (2014), to detect the short-duration pipe burst with a 0.61% false positive in water distribution systems. Xing & Sela (2019) selected SC (Silhouette Coefficient) and CHI (Calinski-Harabasz Index) as the metrics to evaluate K-mean Clustering (KC) performance in clustering time-series water pressure data and they finally identified the number of clusters for the pressure sensor placement. However, it was unclear why they chose these two indexes as the UMLA performance metrics. Previous studies from the computer science field have demonstrated the differences and similarities among the popular performance evaluation indexes such SH, CHI, and DBI (Aggarwal & Zhai 2012; Aranganayagi & Thangavel, 2008; Celebi *et al.* 2013; Cordeiro De Amorim & Mirkin 2012; Xu & Tian 2015). However, there is no systematic study of how these apply to time-series data from UDSs.

We can then define two questions, based on these previous research: 1) Which metrics are the most suitable for assessing cluster model performance based on hydraulic-hydrologic data in UDSs; 2) Which features of these time-series data (length, magnitude, and variability) are the most influential for clustering analysis, and how does the choice of feature affect the clustering solution. To answer these questions, it is necessary to explore how UMLA groups time-series water depth data, and which assessment score can best represent UMLA performance. However, challenges for implementing unsupervised learning algorithms to group the time-series data still exist. Firstly, it is essential to re-format the time-series water depth datasets to make them suitable for clustering. This difficulty is associated with the second research question above since the features of datasets determine how we re-structure the data frame (Mosavi *et al.* 2018; Yaseen *et al.* 2019). Secondly, the connection between the number of clusters and the clustering model performance is another obstacle. As it is still unknown how to correlate clustering performance and the number of clusters in the stormwater urban drainage field, it is required to build such a theoretical relationship for a practical application like outlier detection (Fotovatikhah *et al.* 2018). Therefore, the objective of this study is to improve the understanding of how UMLA facilitates detecting hydraulic anomaly according to the characteristics of water depth datasets in urban drainage networks.

We hypothesize that the performance of clustering algorithms is related to the characteristics of time-series hydraulic data. The layout of the study is as follows: 1) build KC, AC, and SC solutions to group the time-series water depth data; 2) use UMLA metrics such as SCI (Silhouette Coefficient Index), CHI (Calinski-Harabasz Index), and DBI (Davies-Bouldin Index) to evaluate these solutions; 3) compare the best number of clusters obtained by each method; 4) investigate the relationship between model performance and data characteristics. We start by describing the implementation of different UMLA methods, followed by the research methodology with an overview of the real-world case study, performance metrics, and simulation scenarios for cluster analysis. Then we present the results and discussions and, finally, the conclusions.

2. Description of Unsupervised Machine Learning Algorithms

Current machine learning techniques mainly fall into two groups: supervised and unsupervised learning (Kubat 2017). An unsupervised machine learning algorithm (UMLA) is a self-organization method to find patterns in unlabeled data. Cluster analysis is, therefore, a subset of UMLA methods, and in general, is based on the principle of grouping similar observations and segmenting dissimilar observations (Xu & Wunsch 2005). Anomalous data points that differ from others may then be filtered (Shannon 2007). A large number of clustering algorithms exist, including K-means, Affinity Propagation, Mean Shift, DBSCAN, and HDBSCAN. In general, it is difficult to recommend a single algorithm as being the most suitable for clustering, particularly with data that is uncertain and of poor quality, such as the features of drainage data used here (Maier *et al*. 2014; Solomatine and Ostfeld 2008). It is, therefore, advisable to use several algorithms and compare their performance for specific applications. Here, we use K-means, Spectral, and Agglomerative clustering to discover the unknown subgroups in simulated water depth data of UDSs' junctions. Table 1 summarizes the advantages and disadvantages of these algorithms.

Table 1 Clustering algorithm information summary

Models	Definition	Pros	Cons
K-means Clustering	A kind of vector quantization, partition data points into clusters by minimizing the intra-cluster distance.	1)fast, easy-to-understand, and wide applications; 2) stable for time-series data; 3) simple and efficient optimization performance; 4) suitable for huge datasets.	1) number of clusters; 2) spherical assumption.
Agglomerative Clustering	A kind of hierarchical clustering for merging clusters according to a measure of data dissimilarity.	1) stable runs 2) reasonable dendrogram cut-off nodes; 3) clusters growth without globular assumption; 4) good performance for time-series data; 5) no need to know the correct clusters' number.	1) number of clusters; 2) slow implementation; 3) cluster with polluted noise.
Spectral Clustering	A kind of graph clustering based on the distances between points.	1) stable due to the data transformation; 2) no purely globular cluster assumption; 3) easy to implement.	1) number of clusters; 2) slow performance; 3) cluster with polluted noise.

2.1 K-means Clustering

K-means Clustering (KC) is a centroid-based unsupervised clustering algorithm, originally designed for signal processing. It is the most widely applied method of cluster analysis in data mining (Celebi *et al.* 2013). K-means aims to partition the inputs into k partitions. Given a set of observations ($x_1, x_2, ..., x_i$) for p variables, the algorithm runs as follows:

1) Choose k initial centroids, each defined by a value for each of the p variables. These are chosen randomly, often by simply choosing k observations.

2) Assign each observation to the centroid it is most similar to. The similarity is generally measured as the Euclidean distance between the observation and centroid in parameter space.

3) Once all observations are assigned, re-estimate the centroids location as the mean of the p variables of all observations assigned to that centroid.

4) Repeat until the algorithm stabilizes.

The goal then is to minimize $k\mathrm{C}_\ell$the within-cluster sum of squares:

$$\arg min_{\mu,C} \sum_{\ell=1}^{k} \sum_{\mathrm{x_i} \in \mathrm{C}_\ell}^{i} ||\mathrm{x_i} - \mu_\ell||^2 \quad (1)$$

Where k is the number of cluster centers and $\{\mu_\ell\}$, ℓ =1,…k are the cluster centroids $\mathrm{C}_\ell \mu_\ell \mu_\ell \mathrm{C}_\ell$. The total intra-cluster distance is the total squared Euclidean distance from each point to the center of its cluster, and this is a measure of the variance or internal coherence of the clusters (Lloyd 1982). This can be used to assess the stability of the solution. When this falls below a predefined threshold, the algorithm stops. The algorithm is often run multiple times with different random starts to avoid problems in convergence. The clustering solution with the lowest sum-of-squares is chosen as the final output.

However, the choice of *k* is challenging when model performance metrics are not available. Often, an initial value of *k* is chosen, then the algorithm is repeated for higher and lower values. To improve the efficiency of discovering the best k value, a scores-based performance assessment method is recommended in many prior studies (Cordeiro De Amorim & Mirkin 2012).

2.2 Agglomerative Clustering

Agglomerative Clustering (AC) is one of the main forms of hierarchical clustering. These algorithms do not provide a single partitioning of the data but instead provide a full hierarchy of cluster solutions from all observations in a single cluster (i.e. *k=1*) to all observations in individual clusters (i.e. *k=n*) (Rokach & Maimon 2010). In contrast to K-mean, hierarchical methods allow existing clusters to be split or merged, with the result that smaller clusters are related to large clusters in a hierarchy. The rules governing which clusters are again based on their distance or similarity. The AC algorithm consists of the following steps:

1) Start with each data point as its own cluster.

2) Select the distance metric and linkage criteria to calculate the dissimilarity between pairs of observations.

3) Link together the two clusters with the minimum dissimilarity.

4) Continue this process until there is only one cluster.

A key decision in the AC algorithm is the calculation of dissimilarity between clusters. In this study, we used Euclidean distance (Danielsson 1980), and the Ward linkage, which measures the distance between the cluster centroids, similar to the K-means clustering method (Ward 1963). The equations for Euclidean distance and Ward linkage are defined by equation (2) and (3), respectively:

$$||a-b||_2 = \sqrt{\sum_I (a_i - b_i)^2} \tag{2}$$

Where a and b mean the Euclidean vector; a_i and b_i are the point position for the Euclidean vector; i is the number of vectors.

$$d_{ij} = d\big(\{X_i\}, \{X_j\}\big) = ||\mathrm{X_i} - \mathrm{X_j}||^2 \tag{3}$$

Where d_{ij} is the squared Euclidean distance between point i and point j; X_i and X_j are Ward's vectors.

The resulting hierarchy of clusters can be represented using a dendrogram plot (Forina *et al.* 2002). In a dendrogram plot, the y-axis marks the distance at which the clusters merge, while the observations are arranged along the x-axis according to their cluster membership. The dendrogram can then be "cut" at any height on the y-axis to obtain a required number of clusters, with lower heights giving a larger number.

2.3 Spectral Clustering

Spectral Clustering (SC) is an unsupervised learning technique based on graph theory, where SC takes advantage of graph information from the spectrum to find the number of clusters (Von Luxburg 2007). Unlike the previous methods that tend to prioritize clusters by proximity, SC aims to identify observations that are linked, and therefore may not form classical spherical groups in parameter space (Hastie *et al.* 2009). The SC algorithm is as follows:

1) Create a similarity matrix S between observations. This is the complement to the dissimilarity matrices used in other methods, and here is calculated as the negative Euclidean distance.

2) Create an adjacency matrix A, representing the graph or connectivity between observations. This is a transformation of S, where for each observation, we find the k nearest neighbors (i.e., with the highest similarity). If observations i and j are considered to be neighbors, we set $A_{ij} = S_{ij}$. If not, we set $A_{ij} = 0$.

3) Create a degree matrix D, where the diagonal values are the degree of connectivity for each observation, given as $\mathrm{diag}\{D\} = \sum_{i,j}^{n} A_{ij,\ \ i,j=1,2,3,\ldots,n}$

4) Next, calculate the graph Laplacian. This can be normalized or unnormalized. Here, we use the unnormalized: $L = D - A$

5) The clustering solution is then found by eigendecomposition of the Laplacian, and selecting the k smallest eigenvectors. Consequently, these result in a perfect separation of the

observations. K-means is then run on these eigenvectors, to get the final cluster assignment of each observation: $L_{(N\times N)} = \mathrm{D} - \mathrm{A}$

As SC performs dimensionality reduction before clustering data points, it is a very flexible approach for complex data sets. However, the similarity matrix generated by SC may include negative values, which can be problematic for grouping time-series points (Zhang *et al.* 2008).

3. Methods

3.1 Study Area and Data Description

A real-world urban drainage system located in Salt Lake City, Utah, the U.S., was selected as the case study. Due to climate change and urbanization, the studied area has suffered from floods more frequently than before, and the increase in the magnitude and duration of the storm events has pushed the resulting urban drainage out of the pre-defined performance level. Particularly, the flash flooding event on July 26, 2017, which caused millions of dollars of economic loss, was estimated as a 200-year return period storm. This urban drainage network was represented by a rainfall-runoff SWMM (Storm Water Management Model) model. SWMM, which is used throughout the world for planning, analysis, and design related to stormwater runoff, combined and sanitary sewers, and other drainage systems, is a state-of-art tool developed to help support local, state, and national stormwater management objectives to reduce runoff, discharge, and improve stormwater quality (Rossman 2015). Figure.1 shows the components of this SWMM model, which includes one rain gauge, 60 junctions, 61 conduits, two outfalls, and seven sub-catchments.

A total number of 6 artificially designed rainfalls generated by using PCSWMM 7.3 are imported into SWMM as model inputs. Artificial rainfall events are used to test the clustering algorithms as these allow us to control the input and reduce the possible sources of variation between the algorithm results. PCSWMM has its approaches, such as Chicago distribution and SCS distribution, to design rainfall patterns based on precipitation records. For this study, however, we created artificial precipitation series externally and imported them into SWMM within the PCSWMM interface. The distribution for the synthetic rains is shown in Figure.2. These rainfalls have durations of 3 hours, 12 hours, to 48 hours. The return period ranges from 2-year to 5-year. Additionally, rainfall measurements for two real rainfall events were collected to test the clustering algorithm. These rain records are from 2015/05/05 rainfall (3-hour duration) and 2015/07/08 (24-hour duration) rainfall with variable rainfall duration, volume, and intensity. Compared with water depth generated by the artificially designed rainfall data, the time-series water depth produced by the real-world storms is more close to field datasets with non-stationarity and noise.

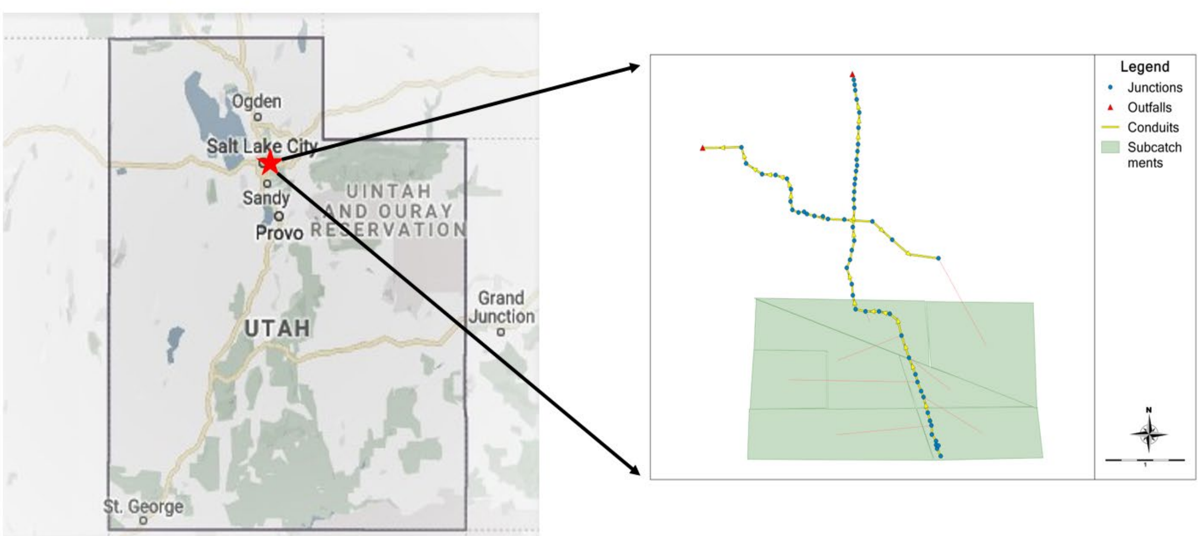


Figure.1. Study area located in the northern Utah state, the U.S. (left subplot: red star), and the topological view of the urban drainage system model plotted by PCSWMM 7.2 (right subplot: scale unit is kilometer).

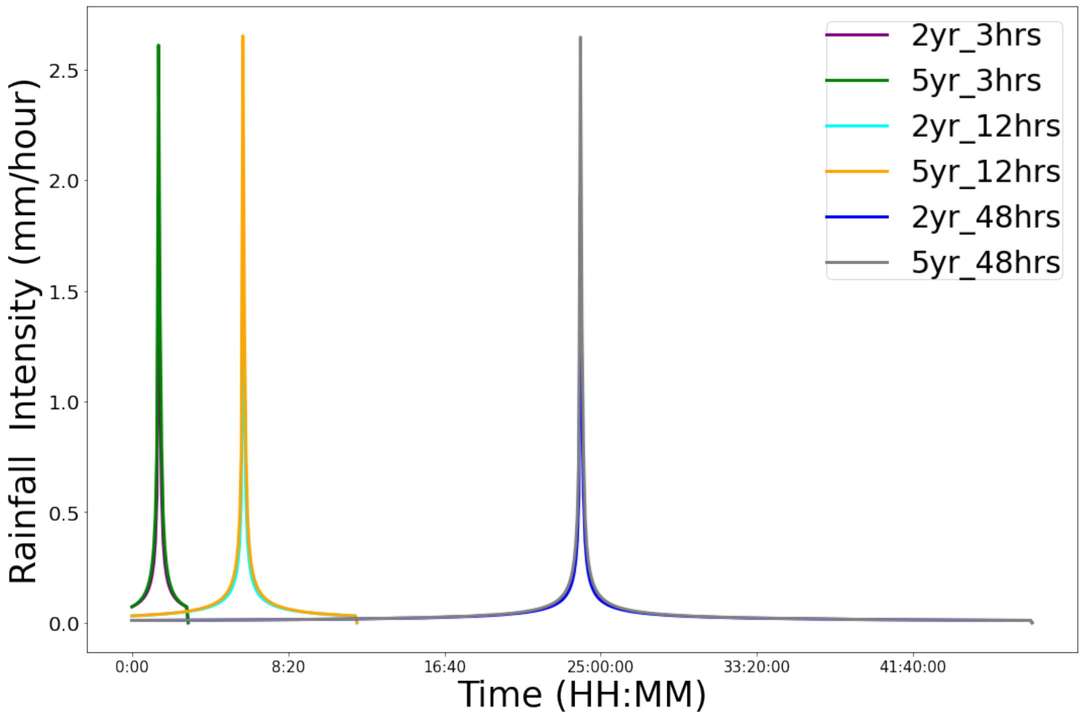


Figure.2. Distribution plots of artificially designed rainfalls with different return periods and rainfall duration, where 'yr' represents the year and 'hrs' stands for hours.

3.2 Clustering Model Implementation

The SWMM model was run six times, once with each of the rainfall scenarios described above. We collected the simulated time-series water depth from each node in the drainage network for cluster analysis. As there are 60 junctions in the SWMM model, this results in a matrix where each column represents a single time step with a 5-minute interval, and each row stands for a junction or node in the network. We then used the principal component analysis (PCA) to reduce the dimensionality of this matrix. PCA uses the eigendecomposition of the correlation matrix to identify a small set of principal components that represent the majority of variance in the original data (Bro and Smilde 2014). Here, we used correlations between the time-series at different nodes to reduce the data from 60 rows to 2. While other techniques for data reduction exist (e.g., correspondence analysis (CCA), factor analysis (FA), or non-metric multi-dimensional scaling

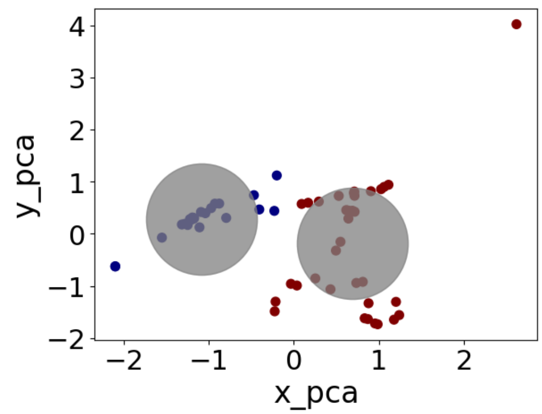
(NMDS)), we used PCA due to the assumed linear response of the water depth values. Although the reduction of dimensionality might cause data loss or an undesirable relationship between axes, it is true that PCA helps reduce computation time and remove redundant data features in the following clustering analysis.

All clustering algorithms were then run using this set of two principal components, with the following set up:

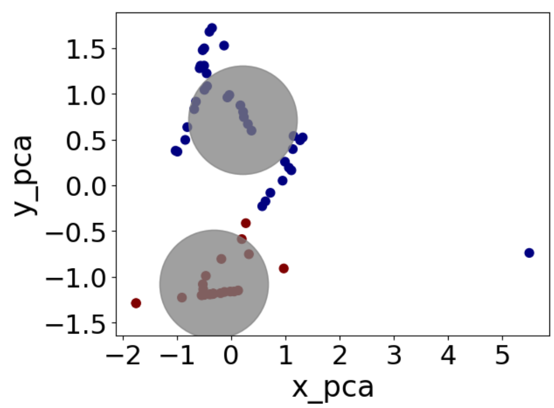
1) K-means: we initially set the number of clusters (k) to 2 for each modeling scenarios, as shown in Figure 2. The algorithm was repeated ten times with different random initialization, and a maximum of 5 iterations was used to converge the algorithm.

2) Agglomerative clustering model: we used Ward linkage, as this is robust to outliers and unequal variance in the data. As only 'Euclidean' supports 'Ward' linkage distance computation. If 'Ward' linkage is used for cluster distance computation, 'Euclidean' would be the best way to measure the data dissimilarity (Pedregosa *et al.* 2011). Thus, the cluster distance calculation method and dissimilarity metric among sample points are set to be 'Ward' and 'Euclidean' distance, respectively. The resulting hierarchy was cut to provide 2 clusters.

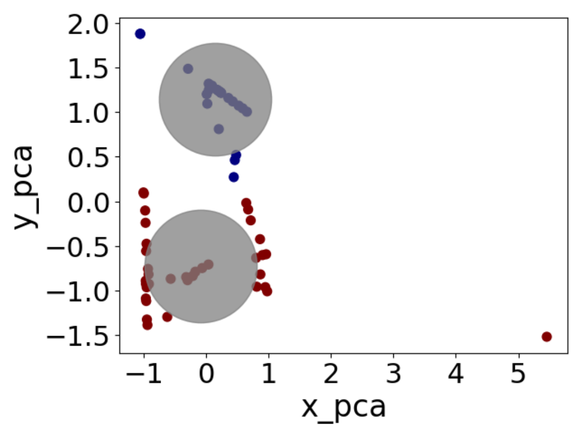
3) Spectral clustering: the algorithm was used to identify 2 clusters, using the unnormalized graph Laplacian


y_pca
4
3
2
1
0
−1
−2
−2
−1
0
1
2
x_pca

(a)


y_pca
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2
−1
0
1
2
3
4
5
x_pca

(b)


y_pca
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1
0
1
2
3
4
5
x_pca

(c)

Figure.3 Datasets (x_pca means the first dimension datasets after principal component analysis; y_pca means the second dimension datasets after principal component analysis) partition by K-mean clustering with 2 clusters (gray circles) under varying rainfall scenarios: a) 3 hours duration rainfall, b) 12 hours duration rainfall, c) 48 hours duration rainfall.

3.3 Clustering Model Evaluation and Validation

Unlike the supervised machine learning algorithm, which can compare the predicted values with the actual values to obtain a measure of model accuracy, UMLA has to assess performance directly on the characteristics of the clusters that were obtained. The performance then depends on data features selected, data preprocessing and parameter settings such as the distance function to use, a density threshold, or the number of expected clusters, which can be modified according to the varying datasets and object inputs. As a result, there is rarely a single obvious solution for clusters, and CA is an iterative process of knowledge discovery or interactive multi-objective optimization that involves trial and failure, aimed to obtain the desired results (Maulik & Bandyopadhyay 2002). Several indices have been proposed to measure the relative performance of different clustering algorithms. In general, these provide an assessment of how the data variance is partitioned. An ideal cluster solution will have low intra-cluster variance (i.e., all observations should be similar within a cluster) and high inter-cluster variance (the clusters should be well separated). Three of these indices are widely used: Silhouette Coefficient (SC), Calinski-Harabasz Index (CHI), and Davies-Bouldin Index (DBI) (Al-Zoubi and Al Rawi 2008; Maulik and Bandyopadhyay 2002; Xiao *et al.* 2017), due to their accuracy and reliability, and we used these here to assess our results.

3.3.1 Silhouette Coefficient Index

The Silhouette Coefficient Index (SCI) is an example of model-self evaluation, where a higher SCI score relates to a model with better-defined clusters (Al-Zoubi & Al Rawi 2008). This score is bounded between -1 for incorrect clustering and +1 for well-formed clusters. Scores around zero indicate overlapping clusters. The SCI is defined for each observation, which can be calculated as equation (5):

$$\mathrm{s} = \frac{m-n}{\max(m,n)} \tag{5}$$

Where the s is SCI for a single observation; m is the mean distance between an observation and all other observations in the same class; n is the mean distance between the same observation and all observations in the next nearest cluster. The SCI has the advantage that it can be used to examine how well individual observations are clustered, or an estimate can be obtained for each cluster or for the whole cluster solution by averaging across a cluster or the entire dataset, respectively. An estimate can be obtained for each cluster or for the whole clusters solution; a set of samples is given as the mean of the SCI for each sample, and it would be relatively higher when clusters are dense and well separated (Aranganayagi & Thangavel 2008).

3.3.2 Calinski-Harabasz Index

The CHI (also known as the Variance Ratio Criterion) is calculated as the ratio of the between-clusters dispersion average and the within-cluster dispersion (Caliñski & Harabasz, 1974), penalized by the number of clusters (k). A higher CHI score indicates better-defined clusters (i.e., dense and well separated). CHI for a set of k clusters is calculated as:

$$\mathrm{s}(k) = \frac{T_r(B_k)}{T_r(W_k)} \times \frac{N-k}{k-1} \tag{6}$$

Where N is the number of points in our data; k is the number of the cluster; T_r represents dispersion matrix; B_k is the between-group dispersion matrix, and W_k is the within-cluster dispersion matrix. B_k and W_k are defined by the following equations:

$$W_k = \sum_{q=1}^{k} \sum_{x \in C_q} (x - c_q)(x - c_q)^T \tag{7}$$

$$B_k = \sum_{q}^{k} n_q (c_q - c)(c_q - c)^T \tag{8}$$

Where C_q is the set of points in the cluster q, c_q is the center of the cluster q, c is the center of the whole data set which has been clustered into k clusters, n_q is the number of points in the cluster q.

3.3.3 Davies-Bouldin Index

Davies-Bouldin Index (DBI) can also be used to evaluate the model, where a lower DBI relates to a model with better separation between the clusters (Davies & Bouldin 1979). The index is defined as the average similarity (R_{ij}) between each cluster and the next closest (i.e., most similar) cluster. The DBI is calculated as equation (9):

$$\mathrm{DB} = \frac{1}{k} \sum_{i=1}^{k} \max_{i \neq j} (R_{ij}) \tag{9}$$

Where DB is the Davies-Bouldin index; Zero is the lowest possible score. Values closer to zero indicate a better partition. k is the number of the cluster; R_{ij} is the similarity measure which features as equation (10)：

$$R_{ij} = \frac{s_i + s_j}{d_{ij}} \tag{10}$$

Where s_i is the average intra-distance between each point of cluster i and the centroid of that cluster representing as cluster diameter; d_{ij} is the inter-cluster distance between cluster centroids i and j; R_{ij} is set to the trade-off between inter-cluster distance and intra-cluster distance. The computation of DBI is simpler than that of SC since this index is computed only with quantities and features inherent to the dataset (Petrovic 2006). However, a good value reported by DBI might not imply the best information retrieval (Xiao *et al.* 2017).

3.3.4 Intra-Cluster Distance

Intra-cluster distance is the distance between two samples belonging to the same cluster. Three types of intra-cluster distance, including complete diameter distance, average diameter distance, and centroid diameter distance, are popular in prior studies. As the number of clusters increase, individual clusters become more homogenous, and the intra-cluster distance decreases. At a certain point, the decrease in distances becomes negligible. Plotting this distance against *k* usually results in an inflection point or elbow where this occurs, and can be used to identify the optimal value of *k* (Thorndike 1953). The number of clusters is chosen at this point, hence the "elbow criterion." Here we use the centroid distance to represent intra-cluster distance, given as double the average distance between all of the objects:

$$\Delta(\mathrm{S}) = 2\left\{\frac{\sum_{x\in S} d(x,T)}{|S|}\right\} \tag{11}$$

$$\mathrm{T} = \frac{1}{|S|}\sum_{x\in S} x \tag{12}$$

Where $\Delta(\mathrm{S})$ is the centroid diameter distance of the formed cluster representative S; x is the samples belonging to cluster S; $d(x,T)$is the distance between two objects, x, and T; |S| is the number of objects in cluster S.

3.3.5 Dendrogram

A dendrogram is a visualization in the form of a tree that shows the hierarchical relationship like the order and distance (dissimilarity) between samples (Stanford 2012). The individual samples are located along the bottom of the dendrogram and referred to leaf nodes. The hierarchical clusters are formed by merging individual samples or existing lower-level clusters. In a dendrogram, the vertical axis is labeled distance and refers to a dissimilarity measure between individual samples or clusters. Generally, in a dendrogram, horizontal lines can be regarded as places where clusters merge, while vertical lines show the distance at which lower-level clusters were merged, forming a new higher-level cluster. The dissimilarity measure between two groups is calculated as equation (13):

$$\mathrm{Dis} = 1 - \mathrm{C} \tag{13}$$

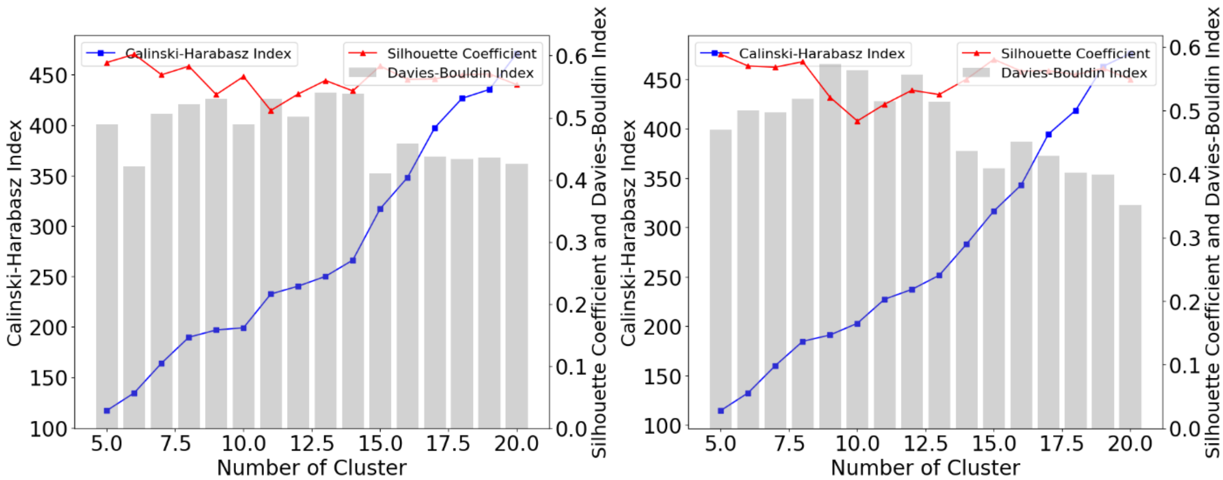
where Dis means the Dissimilarity or Distance among objects; C means the correlation degree between clusters.

If clusters are highly correlated to each other, they will have a correlation value close to 1. To that, Dis =1-C will be given a value close to zero. Therefore, highly related clusters are nearer to the bottom of the dendrogram. Those clusters that are not correlated have a correlation value close to zero. Clusters that are negatively correlated will give a distance value larger than 1 in the dendrogram. The dendrogram can be used to visually allocate correlated objects to clusters or to detect outliers and anomaly in a diagram (Forina *et al.* 2002). In the dendrogram, each sample is treated as a single cluster and then successively combines pairs of clusters until all clusters have been merged into a single cluster. In this process, the dendrogram shows how the aggregations are performed from bottom to top tree statically. This procedure allows the cut-off points to flexibly and efficiently represent the number of clusters. Therefore, this study used the number of cut-off points in the dendrogram to validate the cluster number of the agglomerative clustering.

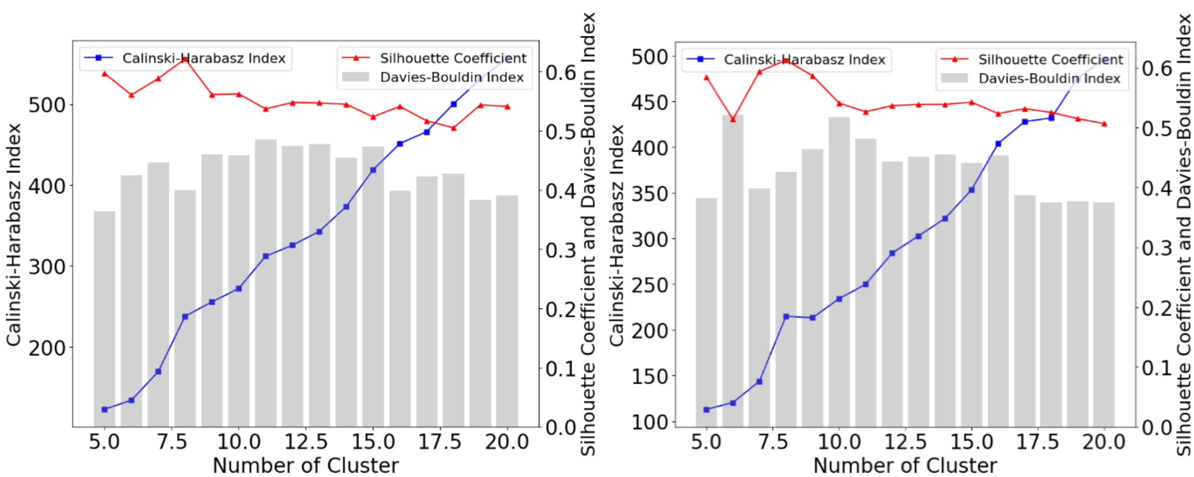
4. Results

4.1 Clustering Performance Evaluation

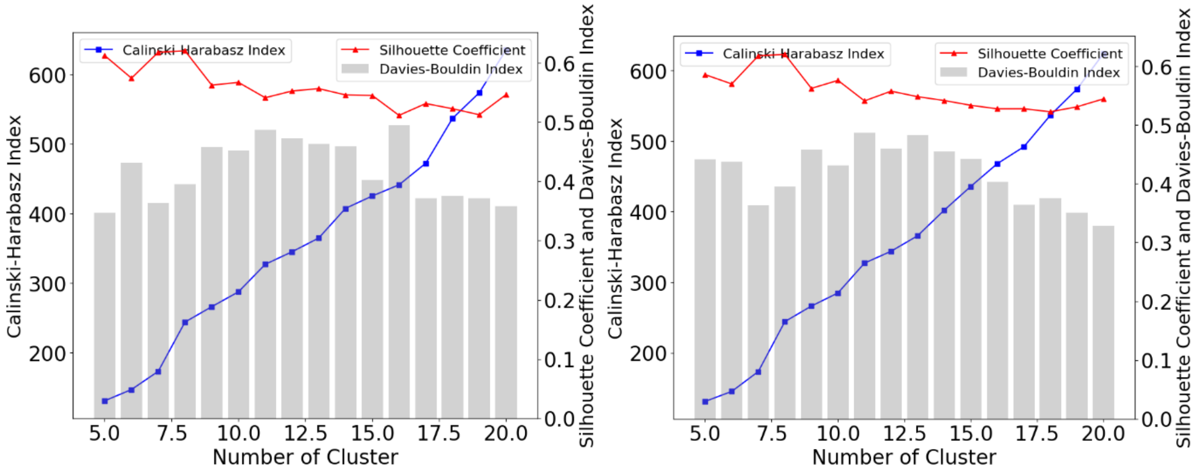
Figure 4 shows how three performance metrics SCI (Silhouette Coefficient Index), CHI (Calinski-Harabasz Index), and DBI (Davies-Bouldin Index) change with different cluster numbers when using K-means to cluster the time-series water depth data. Values for the CHI value increase with higher cluster numbers, whereas the SCI and BDI values fluctuate. The SCI and DBI values show opposite trends, reflecting the different methods by which they are calculated (see above). In particular, Figure.4 b and c show that the best solution is with 8 clusters, reflected in the largest SC value and smallest DBI value. These results suggest that the SCI and DBI are more suitable to assess the performance of K-means, while any peak in the CHI related to cluster quality is eclipsed by the influence of increasing the number of clusters. Based on the SCI and DBI value in Figure.4a, the optimal number of clusters is 6 for the 2year-3hour and 5year-3hour rainfall scenarios. The differences in the optimal number of clusters among Figure.4 a, b, and c indicate that rainfall duration has impacts on the number of clusters when utilizing KC to group time-series water depth datasets.


Calinski-Harabasz Index
Silhouette Coefficient
Davies-Bouldin Index
Calinski-Harabasz Index
Silhouette Coefficient and Davies-Bouldin Index
Number of Cluster
Calinski-Harabasz Index
Silhouette Coefficient
Davies-Bouldin Index
Calinski-Harabasz Index
Silhouette Coefficient and Davies-Bouldin Index
Number of Cluster

(a)


Calinski-Harabasz Index
Silhouette Coefficient
Davies-Bouldin Index
Calinski-Harabasz Index
Silhouette Coefficient and Davies-Bouldin Index
Number of Cluster
Calinski-Harabasz Index
Silhouette Coefficient
Davies-Bouldin Index
Calinski-Harabasz Index
Silhouette Coefficient and Davies-Bouldin Index
Number of Cluster

(b)

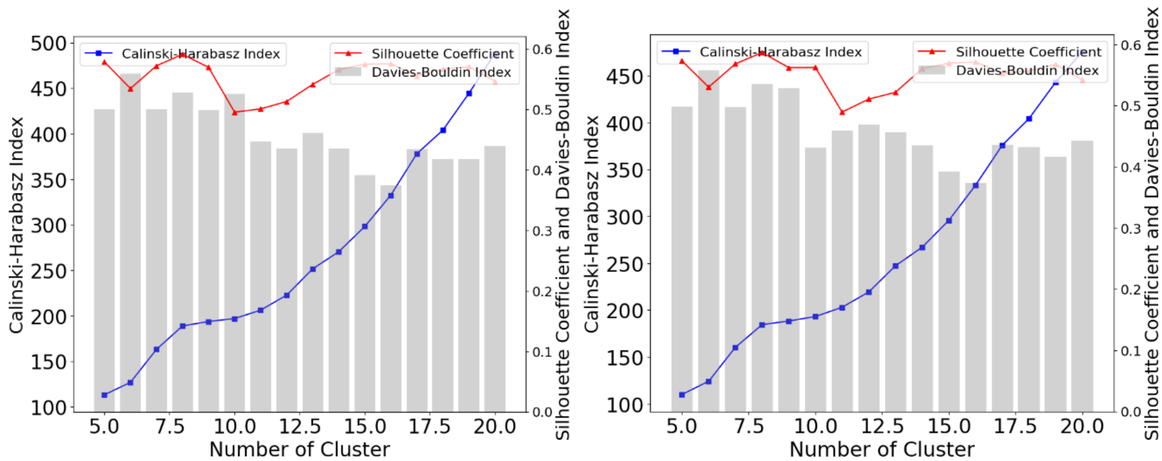


(c)

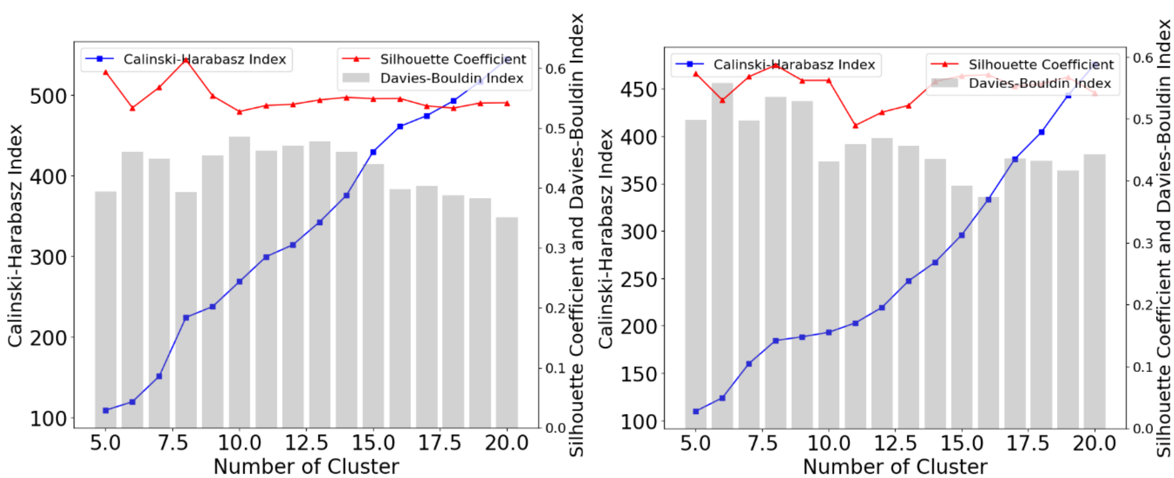
Figure.4. Performance evaluation for K-means Clustering with different cluster numbers under synthetic rainfall scenarios including a) 3-hour (2-year and 5-year), b) 12-hour (2-year and 5-year), and c) 48-hour duration (2-year and 5-year).

Figure 5 shows the same results but based on the use of Agglomerative Clustering to group the time-series water depth data. As with the K-means results (figure 4), the CHI value increase with the number of clusters for all scenarios from short-duration to long-duration rainfall. Again, it is difficult to identify any peak representing an optimal number of clusters, and this suggests that the CHI is not suitable for ascertaining the best clustering solution with these data. In contrast, the SCI and DBI show clear peaks in their values. Figure.5a shows that 16 clusters result in the maximum SCI close to 0.76 and minimum DBI with 0.38. Figure.5c shows a peak in SCI values (~0.6) for 8 clusters, with a corresponding minimum in the DBI value (<0.4). However, Figure.5b shows that 8 clusters could produce the largest SCI (~0.62) and the lowest DBI (~0.40) with the 2year-12hour rainfall duration scenario (left subplot), but that 16 clusters are the optimal solution for the 2yr-12hour rainfall (SCI ~0.58 and DBI ~0.38; right subplot). In summary, the best cluster solutions AC algorithms are 16, 8, and 8 under 3 hours, 12 hours, and 48-hour duration rainfalls, respectively.

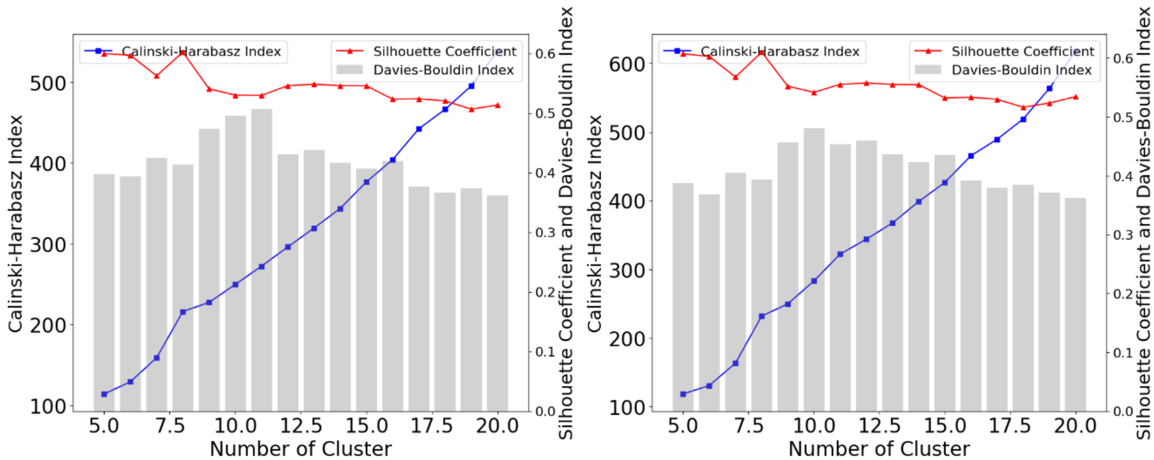
Comparing the left subplots with the right subplots provides (Figure.5) evidence that the cluster number for the best AC performance remains the same, although the return period has been shifted from 2-year to 5-year. The rainfall return period (annual exceedance probability) was found to be less related to the number of clusters.



(a)



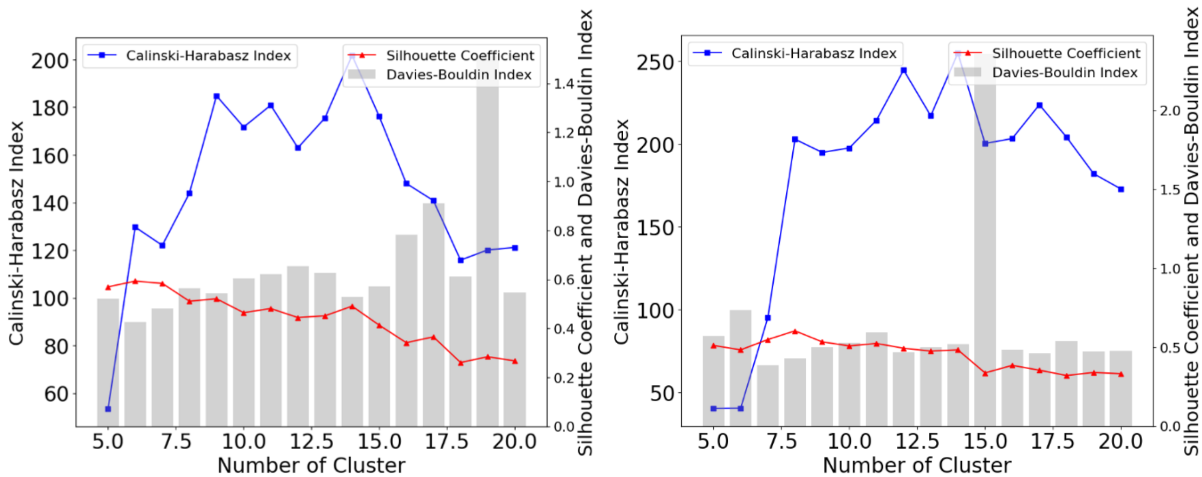
(b)



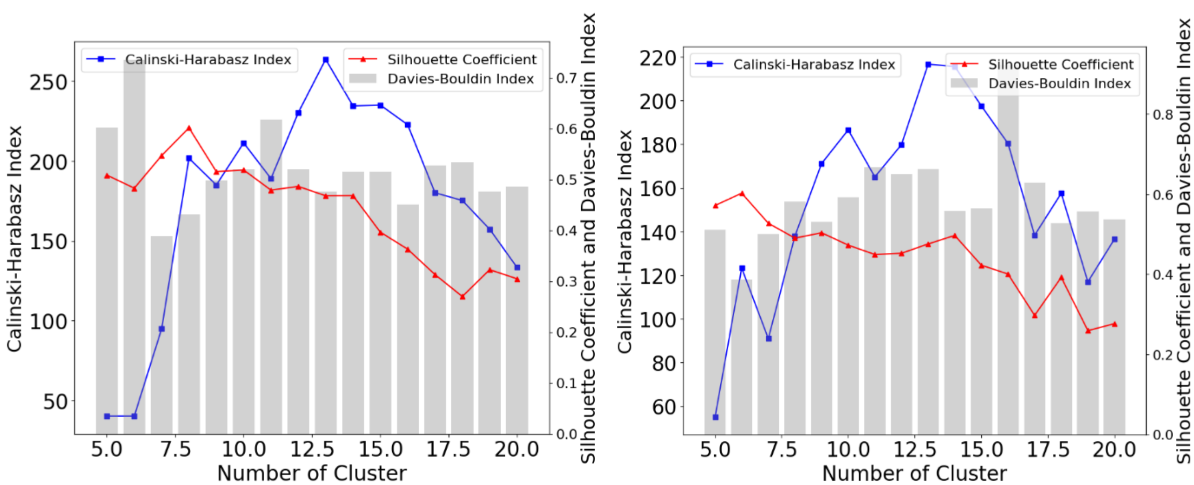
(c)

Figure.5. Performance evaluation for Agglomerative Clustering with different cluster numbers under synthetic rainfall scenarios including a) 3-hour (2-year and 5-year), b) 12-hour (2-year and 5-year), and c) 48-hour duration (2-year and 5-year).

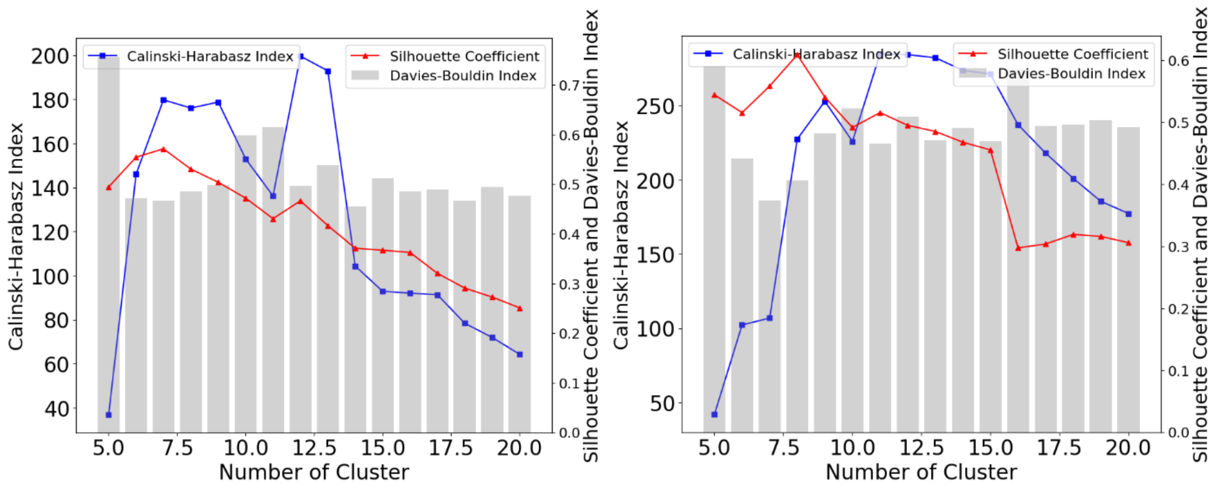
Figure. 6 shows the results obtained for different cluster numbers using Spectral Clustering to group the time-series water depth data. In contrast to the two previous methods, the SCI values decrease as the number of clusters increase. For the 12 and 48 hour scenarios, this index identifies solutions at about 6 to 7 clusters, but no clear optimal solution is identified in the shorter scenarios (panel a). This suggests that this index is unsuitable for assessing this algorithm. The DBI values show greater variation as the number of clusters change, although minima can be observed at 6 to 7 clusters for most scenarios. The CHI values no longer show a linear increase, but show clear peaks, although usually for higher numbers of clusters than the DBI identifies. The highest CHI values (275 for 2 year-12hours and 190 for 5 year-12hours) are all generated by the SC with 13 clusters. For the for 2 year-48 hours and 5 year-48 hours scenarios, the largest CHI values are approximately 200 and 270, respectively, in both cases for 12 clusters.


Calinski-Harabasz Index
Silhouette Coefficient
Davies-Bouldin Index
Calinski-Harabasz Index
Silhouette Coefficient and Davies-Bouldin Index
Number of Cluster

(a)


Calinski-Harabasz Index
Silhouette Coefficient
Davies-Bouldin Index
Calinski-Harabasz Index
Silhouette Coefficient and Davies-Bouldin Index
Number of Cluster

(b)



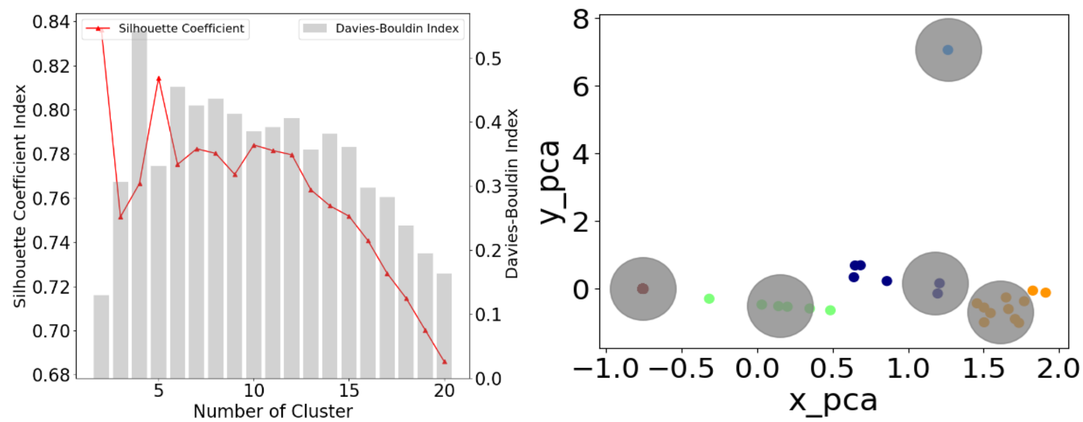
(c)

Figure.6. Performance evaluation for Spectral Clustering with different cluster numbers under synthetic rainfall scenarios including a) 3-hour (2-year and 5-year), b) 12-hour (2-year and 5-year), and c) 48-hour duration (2-year and 5-year).

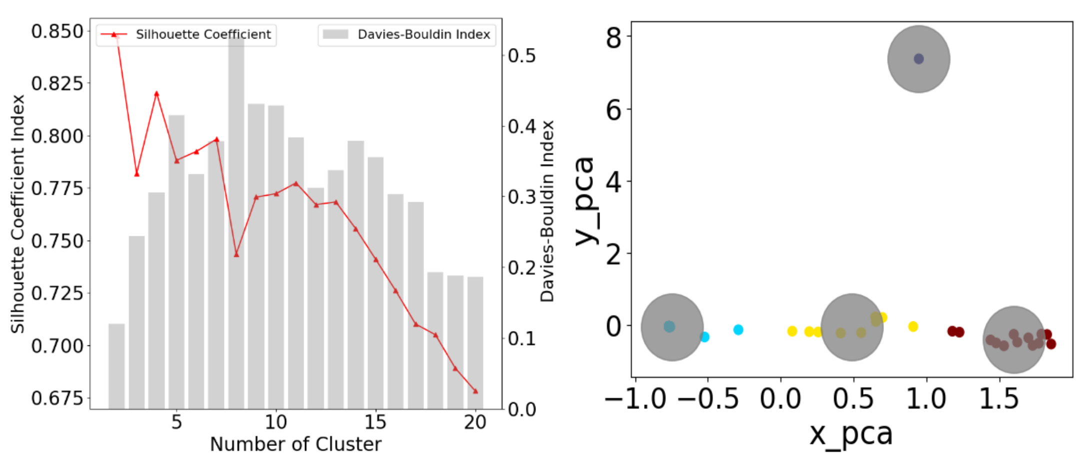
4.2 Clustering Performance Testing

The analysis of cluster performance in the previous section is based on synthetic rainfall datasets, due to the shortage of sensor monitoring for water depth in manholes. However, the use of noise-free synthetic data may have a significant impact on the results obtained (Moazenzadeh *et al.* 2018; Mosavi *et al.* 2018), and our results may not represent real storm situations or currently changing climate conditions. To validate that the results obtained from designed rainfalls can also be applied to non-stationary real-storms, we further investigated the performance of the clustering analysis in grouping water depth datasets generated by two complete rainfall events described below.

The left plots in Figure.7 indicate that the best number of clusters for 2015/05/05 rainfall (Figure 7.a), and 2015/07/08 rainfall (Figure 7.b) are 5 and 4, respectively. Increasing the number of clusters beyond this causes both the SCI and the DBI to decline. The distribution of different clusters obtained is shown in the PCA plots in the right panel of Figure .7. These show that the cluster analysis resulted in a good separation of the storm events (indicated by the lack of overlap between the gray circles). As the rainfall duration increases from 3 hours (the 2015/05/05 storm) to 24 hours (the 2015/07/08 storm), the reduction in the number of clusters selected is in line with the results in section 4, supporting the negative correlation between the number of cluster and rainfall duration.



(a)



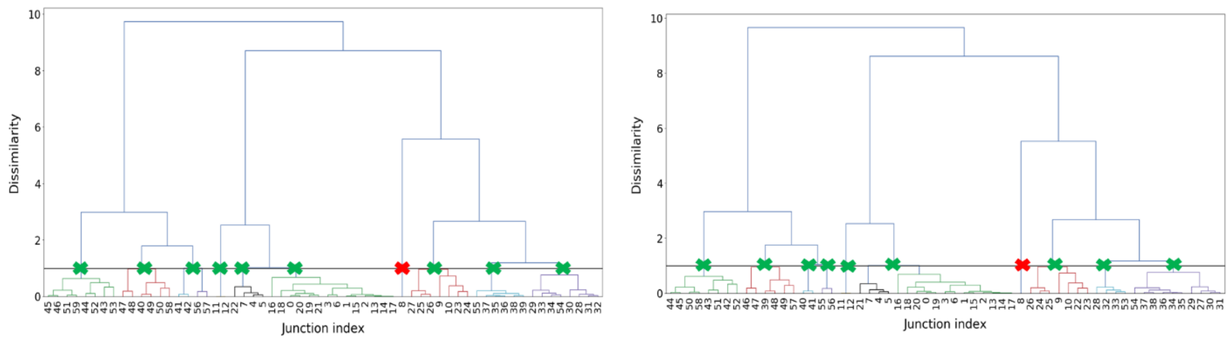
(b)

Figure .7 Clustering analysis test for time-series water depth generated by a) 2015-05-05 storm event; b) 2015-07-08 storm event (gray circles same to clusters).

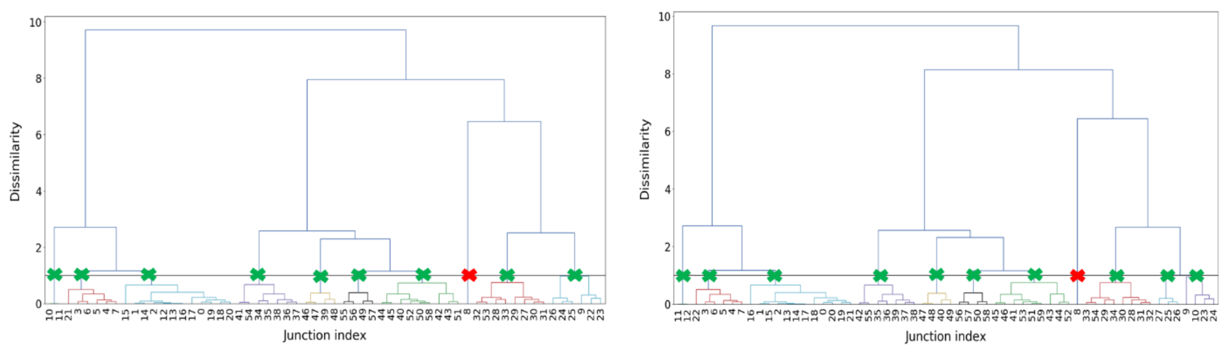
4.3 Cluster Number Validation

Figure.8 shows the dendrogram plots obtained from applying the Agglomerative Clustering algorithm to the observed rainfall data. Generally, the cut-off point should be at least 70% dissimilarity between two clusters or cutting where the dendrogram difference is most significant (Suzuki and Shimodaira 2013). The number of clusters was selected by using a distance threshold of 0.9 distance or 90% dissimilarity, and this is plotted as a horizontal cut-off line in all dendrograms of Figure.8. The cross points (highlighted as green X in dendrogram) between the cut-off line and dendrogram leaves identify the accepted clusters. In Figure.8, one point identified by the cut-off line (junction 8; highlighted as red X in dendrogram) was considered as an outlier in the dendrogram and excluded. In practice, this algorithm might be helpful for anomaly detection in the sensor monitoring network. For instance, real-time monitoring is built to capture the varying different features of measurements as much as possible within a limited number of sensors (Sambito *et al.* 2019). Further, the clusters represent different parts of the hydrological network and can be used to help target locations for sensor deployment to observe overflow and flooding events in the field.

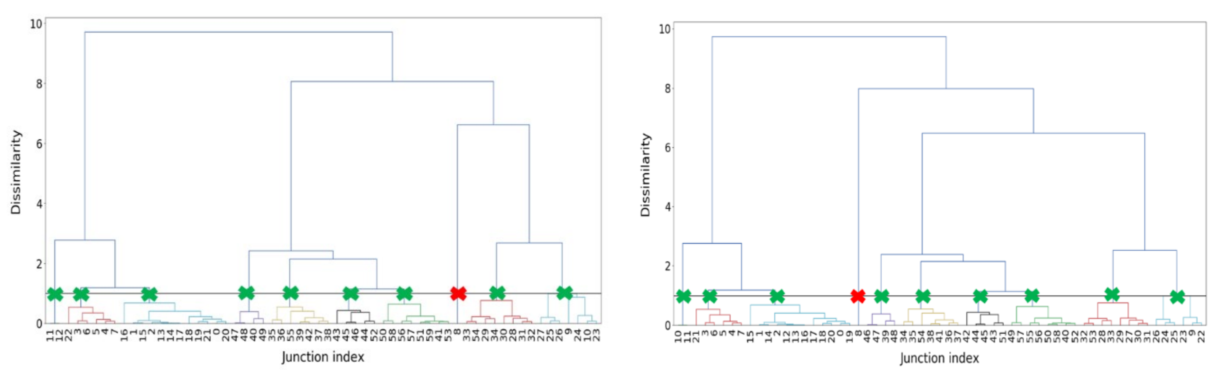
The vertical comparisons among the subplots of Figure.8 (a, b, c) disclosed that the appropriate cluster numbers for 3 hours, 12 hours, and 48 hours rainfall scenarios are quite similar; 8, 9, and 9, respectively. Meanwhile, comparing cluster solutions for different time periods (e.g., left and right plot of Figure.8a), the number of clusters and their structure is remarkably similar, implying that the rainfall return period has fewer impacts on AC model performance. This supports the conclusions reached with the synthetic time series, that the AC model performance noticeably depends on the rainfall duration but not the rainfall return period (exceedance probability).



(a: left 2year-3hours; right 5year-3hours)



(b: left 2year-12hours; right 5year-12hours)



(c: left 2year-48hours; right 5year-48hours)

Figure.8 Dendrogram (green X representing acceptable cluster; red X representing unacceptable X) for comparing agglomerative cluster numbers between 2-year return period (the left subplots) and 5-year return period (the right subplots) rainfall scenarios.

This study adopted intra-cluster distance as the metric to assess the effects of rainfall duration and return period (exceedance probability) on the performance of the K-means and Spectral Clustering algorithm. Figure.9 shows the results of this comparison, with the decay in the intra-cluster distance as the number of clusters increases. A notable elbow can be seen above 4 clusters, as the decrease in distances becomes much smaller. Using the elbow criterion described in section 3.3.4, this suggests that 4 clusters are the best solution. Increasing the number of clusters beyond this would result in a little additional gain for the extra complexity of the solution. Figure.9 shows that the intra-cluster distance changes in a similar way for all six rainfall scenarios, and that the intra-cluster distance is identical in those rainfalls with the same duration. For example, the solid purple line with purple circle markers (representing 2 year-3 hours rainfall scenario) overlaps the red dashed line with the red circle markers (representing 5 year-3 hours rainfall scenario). However, there are still some differences between scenarios with different rainfall duration. Notably, the intra-cluster distance increases as the rainfall duration decreases (the distance for the '3hrs' duration rainfall is the largest, followed by the '12hrs' cases, and then the '48hrs' scenarios). As a metric for clustering performance, intra-cluster distance is therefore useful in determining how well these algorithms group the water depth time-series. These results suggest that the K-means and Spectral Clustering algorithms work best with longer duration rainfalls. This suggests that the longer duration rainfall results in greater similarity in the flow at different junctions. This, coupled with the larger set of observations from a longer period, results in better formed individual clusters. Shende and Chau (2019) have shown that these cluster methods work optimally when trained on massive datasets, which is supported by our results herein.

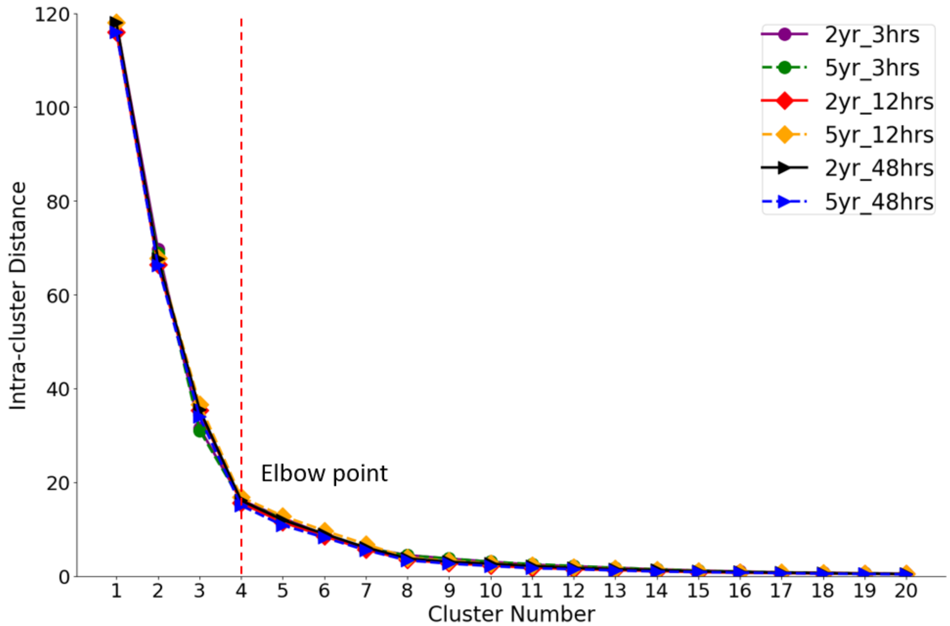


Figure.9 Cluster Intra-distance for comparing the effects of rainfall duration and return period on the performance of K-means and Spectral model (elbow point is the cross between the red dash-line and curves) under 6 synthetic rainfall scenarios (‘yr’ represents year while ‘hrs’ stands for hours).

5. Discussions

In this study, we used unsupervised machine learning algorithms to group simulated time-series water depth of urban drainage systems under six synthetic rainfalls and two measured storms. We applied three different algorithms (K-means clustering, Agglomerative clustering, and Spectral clustering), and evaluated the results using three indices (Silhouette Coefficient, Calinski-Harabasz Index, and Davies-Bouldin Index). These results provide a better theoretical understanding of the different methods, how to use them with these data, and which metrics are suitable for assessing the cluster solutions. We also demonstrate how the characteristics of the dataset (notably length and magnitude) influence the number of clusters. This information should help facilitate the detection of urban flooding events using water depth datasets in real drainage networks (Chang *et al.* 2010; Guo *et al.* 2018).

Previous cluster-based studies have mainly focused on detecting pressure, demand, pipe burst, infrastructure damage, and illicit intrusion in water distribution systems (Perelman and Ostfeld 2012; Sambito *et al*. 2019; Wu and Liu 2020; Xing and Sela 2019). In the clustering analysis here, the features, such as the length of time-series water depth from UDSs, are found to be negatively correlated with the number of clusters. This finding has been validated by the dendrogram cut-off points in designed rainfalls and also by the cluster center mapping based on real storm events. The similar results between the artificial (noise-free) and practical (noise-polluted) scenario infer that modeling duration (data length) overwhelms the event exceedance probability (data magnitude) in the cluster number identification, which agrees with the findings from Wu *et al*. 2016. Increasing the number of clusters often results in many more errors. One extreme case is that the zero error happens when each data point is equal to every cluster. Intuitively, the choice of the best number of clusters can be interpreted into a trade-off between maximum compression of the data with a single cluster and maximum accuracy by assigning each data point to its cluster (WIKIPEDIA 2015).

In addition to the cluster number determination, the structure of datasets may also affect the clustering model performance. K-means and Spectral Clustering algorithms are able to robustly group water depth datasets from longer duration rainfall events. However, there is little relationship between algorithm performance and annual exceedance probability. The sharply rising trend (Figure.4 to Figure.6) demonstrates that the CHI is not suitable to identify the best number of clusters in the K-means and Agglomerative Clustering algorithms, but that the SCI and DBI work quite well and give comparable results (Figures 4, 5 and 6). In contrast, the CHI works well in identifying the optimal cluster number with the Spectral Clustering algorithm. This difference reflects the different nature of the algorithms: K-means and Agglomerative Clustering are based on simple dissimilarity measures between observations, whereas the Spectral Clustering is based on a graph representing connectivity. This is because that DBI evaluates intra-cluster similarity among every data point and inter-cluster differences among each group. Similarly, the SCI measures the distance between each data point and the centroid of the cluster it was assigned to. An SCI value close to 1 is always good, and a DBI value close to 0 is also good whatever clustering you are trying to evaluate. However, the CHI is not normalized, and it's difficult to compare two values of the CHI index from different data sets.

Although this study has identified some clear differences in the application of cluster analysis, there are several limitations. Firstly, the majority of scenarios used time-series water depth datasets generated by model simulation. As these are smooth and noise-free, the results may not scale to field application. However, we found similarities between the results with the limited set of observed rainfall series used here, notably in the use of the different indices, but tend to result in a smaller number of clusters. Further work should apply these methods to a wider set of observed data if such data becomes available. Secondly, this paper only focuses on clustering model implementation and performance evaluation. Future work will concentrate on the application of these methods, including sensor placement, overflow detection, and flooding monitoring. Since the dendrogram enables the AC algorithm to detect outliers in time-series water depth datasets, this can be used to help guide sensor deployment for observing overflow and flooding forecasting in the field (Panganiban and Cruz 2017). It is planned to consider strengthening the connection between the theoretical results and field application by conducting a clustering analysis to optimize the sensor monitoring network for flooding detection at UDSs.

6. Conclusions

In the age of 'Smart Stormwater,' the increased deployment of sensors to monitor flow characteristics is resulting in rapidly accumulating data. It is becoming crucial to understand and promote methods to handle these big datasets to help in flood monitoring and forecasting. This study aims to promote understanding of how clustering analysis facilitates the interpretation of the unlabeled time-series water depth data for flood detection at urban drainage systems. In this work, three indexes, including Silhouette Coefficient Index, Calinski-Harabasz Index, and Davies-Bouldin Index, were used to evaluate the performance of three popular unsupervised clustering analysis models namely K-means clustering, Agglomerative clustering, and Spectral clustering. A real-world urban drainage systems SWMM model was applied to generate the time-series water depth under six rainfall scenarios and two real rainstorms. Four conclusions were drawn below:

(1) Silhouette Coefficient Index and Davies-Bouldin Index are suitable metrics to measure the performance of K-means and Agglomerative clustering model when subject to identify the number of clusters for the best performance. However, Calinski-Harabasz Index is found to be more favorable to assess the performance of the Spectral clustering model in grouping time-series water depth datasets.

(2) In K-means and Spectral clustering models, the number of the clusters for maximizing model performance is highly related to the dataset length (simulation duration) but is slightly associated with the dataset magnitude. There is a negative correlation between the number of clusters and the length of datasets (modeling timesteps).

(3) The short-period water depth data can be well-grouped by the Agglomerative clustering model. In contrast, K-means and Spectral clustering models are more able to handle time-

series water depth datasets from long-duration storm scenarios.

(4) This research work provides insight into unlabeled hydraulic data-driven techniques by conducting clustering experiments. The outcomes are useful for researchers to select the appropriate clustering model and to choose the corresponding performance metrics for specific case applications.

Declarations of interest

None

Acknowledgments

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