Abstract—This paper presents noise-robust clustering techniques in unsupervised machine learning. The uncertainty about the noise, consistency, and other ambiguities can become severe obstacles in data analytics. As a result, data quality, cleansing, management, and governance remain critical disciplines when working with Big Data. With this complexity, it is no longer sufficient to treat data deterministically as in a classical setting, and it becomes meaningful to account for noise distribution and its impact on data sample values. Classical clustering methods group data into “similarity classes” depending on their relative distances or similarities in the underlying space. This paper addressed this problem via the extension of classical $K$-means and $K$-medoids clustering over data distributions (rather than the raw data). This involves measuring distances among distributions using two types of measures: the optimal mass transport (also called Wasserstein distance, denoted $W_2$) and a novel distance measure proposed in this paper, the expected value of random variable distance (denoted ED). The presented distribution-based $K$-means and $K$-medoids algorithms cluster the data distributions first and then assign each raw data to the cluster of data’s distribution. These noise-robust clustering algorithms have been implemented in MatLab and applied to cluster noisy real-world weather data by efficiently extracting and using underlying uncertainty information (means and variances). The results on weather data show striking improvement in performance for $W_2$ and ED distance-based $K$-means and $K$-medoids, and where higher accuracy is observed for ED compared to $W_2$ for both $K$-means and $K$-medoids. This is because while $W_2$ works with marginal distributions ignoring the actual correlations in computing the distance measure, ED works with the joint distributions factoring the correlations into the distance measurements.

Index Terms—Clustering algorithms, Expectation distance, Wasserstein distance, Uncertain data

I. INTRODUCTION

DATA is naturally and inherently affected by the random nature of the physical data generation process and measurement inaccuracies, $[1]–[3]$, sampling discrepancy, outdated data sources, or other errors, making it prone to noise/uncertainty. These several sources of uncertainty have to be accounted for in order to produce accurate classification/regression results. Clustering, a widely studied unsupervised learning technique, is commonly used in many fields for statistical data analysis to make valuable inferences from data by observing what groups each data point falls into. Classical clustering methods, such as the two popular partition-based methods of clustering, $K$-means and $K$-medoids clustering, group data into “similarity classes” depending on their relative distances or similarities in the underlying space. A widely used example of the similarity measure among data would be the euclidean distance. The main aim of clustering is to partition the data points into clusters so that the data’s total distance (commonly the euclidean distance) to their assigned cluster centers is minimized $[4]$. Iterative clustering algorithms have been devised to perform clustering efficiently, which utilizes only the raw data without requiring any additional information about the data (such as labels). Although very efficient, the classical algorithms were not designed to address situations where the data is uncertain/noisy. One viable way to minimize the effect of uncertainty in data is to utilize its probability distribution (if it can be estimated); cluster the distributions, and assign raw data to its distribution cluster—This way, the chances of an outlier data getting wrongly assigned to an incorrect cluster is reduced.

Clustering uncertain data has been well-recognized as a challenge in the data mining fields $[5]$. An example of an uncertain data source is data from sensor networks that are typically subject to sensor noise. As an application of clustering uncertain data according to their probability distributions, consider a weather station that monitors and measures daily the variables like temperature, humidity, and vapor pressure, amongst other important factors. The data is inherently uncertain and naturally noisy, and uncertain due to physical measurement equipment (backed by thermal noise and Heisenberg’s Uncertainty Principle) and daily thermal and other noise variations as a result of natural weather changes. While it is expected that the daily weather conditions are within specific predicted ranges for certain seasons, there are cases and days where this may vary. Due to these, the weather record can be modeled as an uncertainty represented by a distribution over the space formed by several measurements. We may group the weather conditions during each month or season for stations in a particular region. Under the presence of such uncertainty, it is no longer sufficient to treat data deterministically as in a classical setting, and it becomes meaningful to account for noise distribution and its impact on data sample values. A probability distribution can generally represent uncertain data $[5]–[8]$, which may then be used towards a more noise-robust clustering for better accuracy $[4]$.

A. Our Contributions

This paper addresses the issues of clustering uncertain data with the following contributions:

- We propose a new distance measure, Expectation Distance (ED), among the distributions, which overcomes the limitations of the widely-used $W_2$. We make the observation that the $W_2$ distance only depends on the pairwise marginal distributions, ignoring the true correlation information. In contrast, the proposed ED overcomes this limitation by factoring in the correlation information.

This work has been submitted to the IEEE for possible publication. Copyright may be transferred without notice, after which this version may no longer be accessible.
and, in the process, yields more noise-robust clustering results. We have shown that ED meets all the required criteria of a statistical metric (positivity, symmetry, triangular inequality, and zero if and only if equal). ED can be utilized in other machine learning cases where distances are required to obtain noise-robust results.

- We formulate distribution distance-based noise-robust clustering algorithms, efficiently extracting and using the underlying uncertainty information (e.g., means and variances) to cluster noisy real-world data. These algorithms are derived by extending the classical clustering techniques of K-means and K-medoids to cluster over the data distributions (rather the raw data), and measuring distances among distributions by exploring two types of statistical distance measures: Optimal Mass Transport, OMT (also called Wasserstein distance, denoted $W_2$), and the proposed the Expectation Distance (denoted ED) of the random variable distance. The presented distribution-based K-means and K-medoids cluster the data distributions first and then assign each raw data to the cluster of its distribution.

- While the Barycenters, whose calculation does not require distance measure, serve as the cluster-centers in both K-means algorithms ($W_2$-based vs. ED-based), the cluster-centers for the K-medoids differ in the $W_2$-based vs. ED-based distances. In all cases, the clustering accuracy (whenever the ground truth is known as in the case of the weather seasons) is higher for distribution distance-based clustering compared to raw-data clustering, and further, the ED distance-based clustering is more accurate than the $W_2$ distance-based clustering. This later enhanced robustness of ED over $W_2$ is because the former also depends on joint distributions factoring in the correlations, while the latter only depends on the marginal distributions ignoring the correlations.

- We implement, apply, and compare all six clustering algorithms (K-means and K-medoids for deterministic vs. $W_2$-based vs. ED-based distance measures) to noisy real-world weather data and show that the results demonstrate a striking improvement in performance for $W_2$ and ED distance-based K-means and K-medoids compared to the classical clustering of raw-data. Additionally, in both K-means and K-medoids, the ED-based measurement offers higher accuracy than the $W_2$ based distance for the reason mentioned in the previous item.

B. Related works

In general, uncertain data, which can be statistically defined as data that contains noise that makes it deviate from the correct, intended, or original value, can be classified into existential uncertainty and value uncertainty (also called attribute level) [11, 12, 14, 9]. Existential uncertainty exists when it is uncertain about whether a data tuple is in an uncertain database and is usually represented by a probability that represents the confidence of its presence. The presence and absence of one tuple may affect the probability of the presence or absence of another tuple in the database. Value uncertainty appears when a tuple is known to exist with some of its attributes are partially known [10]. Data with value uncertainty is represented by standard error of individual data [11, 2], probability density functions [12, 13] or probability distribution function [14].

Cluster analysis is a well-researched field in machine learning fields. There are some existing studies: The classical DBSCAN (Density-Based Spatial Clustering of Applications with Noise) [15], and OPTICS (Ordering Points To Identify the Clustering Structure) [16] have also been extended [17, 18] in a probabilistic way where objects in geometrically dense regions are grouped as clusters and clusters are separated by sparse regions. However, when objects heavily overlap, and there are no apparent sparse regions to separate objects into clusters, these approaches fail to work well.

The Optimal Mass Transport (OMT) has been used in several applications ranging from classical ML (clustering, classification, and PCA) to state-of-the-art learning techniques (GAN, Deep Learning). $W_2$ is a distance function defined between probability distributions. It uses the Optimal Mass Transport (OMT) concept in defining a distance metric between a pair of probability distributions of two random variables. The cost among all possible transports would need to be minimized to find the OMT distance. When the cost of transportation is the square of the Euclidean distance between their support points, OMT results in a Euclidean-like geometry on probability densities. It equips the space of probability densities with a Riemannian metric. The resulting geometry is then used as a tool to formulate geodesic paths. The metric induced by the cost of transport is called the Wasserstein $W_2$-distance [19]. In [20], the authors developed clustering algorithms to cluster measure-valued data with the Wasserstein distance. In this paper, we have further extended the Wasserstein distance-based clustering algorithm to the case of K-medoids.

Another initial extension of K-means to stochastic setting is $U/K$-means considered in [21] and subsequently used in [12, 13], that takes the cluster-center to be the average of the means of distribution data, i.e., for a cluster $C$ its cluster-center is taken to be: $c = \frac{1}{|C|} \sum_{x \in C} E(x)$. The distance between a distribution data $x$ and a cluster-center $c$ is taken to be the Expectation Distance, $E(\|c - x\|^2) = \|c - E(x)\|^2 + tr(\Sigma_C)$. Thus $U/K$-means limits itself by taking the cluster center to be deterministic; namely, the average of the data means, which is not the case in our study and instead the cluster-center is also a distribution (the Barycenter in case of K-means and one of the distribution data in K-medoids).

II. NOISE-ROBUST CLUSTERING

A. Clustering

Consider a set $X$ that needs to be clustered into $K$ number of clusters. Then the clustering problem requires finding a function $C : X \rightarrow [1, K]$ to map each element of $X$ to one of the $K$ clusters in some optimal sense. Then for each $i \in [1, K]$, the $i^{th}$ cluster under the clustering $C$ is given by

$$X_C(i) := \{x \in X | C(x) = i\},$$

(1)
and its cluster-center (also called Barycenter) is the center-of-mass of the cluster elements:

\[ \hat{x}_C(i) := \frac{\sum_{x \in X_C(i)} x}{|X_C(i)|}, \forall i \in [1, K]. \] (2)

Note that \( \hat{x}_C(i) \) is also the minimizer of the distance:

\[ \hat{x}_C(i) := \arg \min_{x} \sum_{x' \in X_C(i)} |x - x'|, \forall i \in [1, K]. \] (3)

The goal is to find an optimal \( K \)-cluster that minimizes the aggregate distances of each of the elements to their respective cluster-center, i.e.,

\[ \min_C \sum_{i=1}^{K} \sum_{x \in X_C(i)} |\hat{x}_C(i) - x'| \]

where the notation \(|.|\) measures the length of its argument vector or the size of its argument set. The corresponding optimal cluster is called \( K \)-means. Note that for \( K \)-means, a cluster-center is a Barycenter and may not coincide with any of the data points. If we require the cluster-center be always one of the data points, then the resulting clustering algorithm is called \( K \)-medoids for which the objective function can be written as:

\[ \min_C \sum_{i=1}^{K} \min_{x \in X_C(i)} \left( \sum_{x' \in X_C(i)} |x - x'| \right) \] (4)

Here the inner optimization minimizes the distance between one data point in a cluster to all other data points within the same cluster to find a cluster-center:

\[ \hat{x}_C(i) := \arg \min_{x \in X_C(i)} \sum_{x' \in X_C(i)} |x - x'|, \forall i \in [1, K]. \] (5)

Note in contrast to (3), the minimization in (6) is restricted to over the set \( X_C(i) \).

One popular heuristic to find a local optimal \( K \)-means cluster involves starting with an arbitrary initial cluster \( C_0 \), and iteratively finding a better cluster \( C_{n+1} \) from a prior cluster \( C_n \), \( (n \geq 0) \), until this process converges, i.e., until \( C_{n+1} = C_n \). The heuristic finds the \( i^{th} \) cluster of the \( (n+1)^{th} \) iteration as the set of elements that are nearest to the \( i^{th} \) cluster-center of the \( n^{th} \) iteration. The same iterative computation for \( K \)-means can be used to find \( K \)-medoids with the change that the revised definition of cluster-center is used.

To extend the \( K \)-Means and \( K \)-medoids and make those robust with respect to noise outliers, we propose clustering over the data distributions (as opposed to raw data) and then assigning each raw data to the cluster of its distribution. This way, the effect of outliers is reduced, making the clustering more noise-robust. Clustering over distributions requires measuring distances between pairs of those, and for this, we consider the commonly used Optimal Mass Transport (OMT) and the Expectation Distance (ED) that we propose for the first time.

### B. Optimal Mass Transport/Wasserstein Distance Formulation

OMT computes the distance between two distributions \( \mu_X \) and \( \mu_Y \) of two random variables \( X \) and \( Y \), respectively, by associating cost to “transport” the probability mass from the starting distribution \( \mu_X \) to the destination distribution \( \mu_Y \), and minimizing that cost. The \( W_2 \)-metric is weakly continuous, such that its convergence in the metric is equivalent to the convergence of moments [22].

Letting \( T : \mathbb{R}^n \rightarrow \mathbb{R}^n \) denote a transport map, OMT minimizes the associated cost of transport:

\[ \min_T \int_{\mathbb{R}^n} c(x, T(x)) \mu_X(dx). \] (7)

Kantorovich proposed the cost to be Euclidean distance, \( c(x, T(x)) = ||x - T(x)||^2 \), and looked to minimize the transport cost over the joint distributions \( \pi \in \prod(\mu_X, \mu_Y) \) on \( \mathbb{R}^n \times \mathbb{R}^n \) so that the marginals along the two coordinate directions coincide with \( \mu_X \) and \( \mu_Y \) respectively [23]:

\[ W_2^2(\mu_X, \mu_Y) := \inf_{\pi \in \prod(\mu_X, \mu_Y)} \int_{\mathbb{R}^n \times \mathbb{R}^n} ||x - y||^2 \pi(dx, dy). \] (8)

1) **Cluster-center:** The cluster-center for a cluster \( C \) in case of \( K \)-means is given by:

\[ \arg \min_{\mu'} \sum_{\mu \in C} W_2^2(\mu', \mu). \] (9)

The cluster-center turns to be the Barycenter \( \frac{1}{|C|} \sum_{\mu \in C} \mu \) [20].

In contrast, in the case of \( K \)-medoids, a cluster-center is chosen to be one of the data points, and so their joint distribution is already estimated from the data (and it is no longer an optimization variable as in the case of \( K \)-means):

\[ \arg \min_{\mu' \in C} \sum_{\mu \in C} W_2^2(\mu', \mu). \] (10)

2) **OMT measure and OMT-based Barycenter for Gaussian distributions:** Gaussian noise is the most common type of noise in the physical world and is particularly useful in developing concepts. When the randomness can be modeled as Gaussian distributions, say, \( \mu_X \equiv \mathcal{N}(m_X, \Sigma_X) \) and \( \mu_Y \equiv \mathcal{N}(m_Y, \Sigma_Y) \), there exists a closed-form expression of their \( W_2 \) distance and Barycenter, as discussed below. Letting \( \bar{X} = X - m_X \) and \( \bar{Y} = Y - m_Y \) denote the zero mean equivalent of \( X \) and \( Y \) respectively, we have:

\[ \int_{\mathbb{R}^n \times \mathbb{R}^n} ||x - y||^2 \pi(dx, dy) = \mathbb{E}[||\bar{X} - \bar{Y}||^2] \]

\[ = \mathbb{E}[||\bar{X} + m_X - (\bar{Y} + m_Y)||^2] \]

\[ = \mathbb{E}[||\bar{X} - (\bar{Y} + m_Y)||^2 + ||m_X - m_Y||^2] \]

\[ = \text{trace}(\Sigma_X + \Sigma_Y - 2\Sigma_{XY}) + ||m_X - m_Y||^2, \]

where \( \Sigma_X = \mathbb{E}[\bar{X}\bar{X}^T], \Sigma_Y = \mathbb{E}[\bar{Y}\bar{Y}^T], \Sigma_{XY} = \mathbb{E}[\bar{X}\bar{Y}^T]. \) The minimization of (11) then yields a semidefinite program:

\[ \min_{\Sigma_{XY}} \left[ \text{trace}(\Sigma_X + \Sigma_Y - 2\Sigma_{XY}) + ||m_X - m_Y||^2 \right] \]

s.t. \[ \begin{bmatrix} \Sigma_X & \Sigma_{XY} \\ \Sigma_{XY}^T & \Sigma_Y \end{bmatrix} \succeq 0. \] (12)
The minimum in (12) is achieved at:
\[ \Sigma_{XY} = (\Sigma_X^{1/2} \Sigma_Y \Sigma_X^{1/2})^{1/2}. \] (13)
Thus the \(W_2\) distance for the Gaussian distributions satisfies:
\[ W_2^2(\mu_X, \mu_Y) = ||m_X - m_Y||^2 \\
+ tr[\Sigma_X + \Sigma_Y - 2(\Sigma_X^{1/2} \Sigma_Y \Sigma_X^{1/2})^{1/2}]. \] (14)

For Gaussian distributions \(\{\mu_k = \mathcal{N}(m_k, \Sigma_k), 1 \leq k \leq K\}\), the Barycenter is also Gaussian with its mean and covariance matrix, \(m\) and \(\Sigma\) respectively, satisfying [22]:
\[ m = \frac{1}{K} \sum_{k=1}^{K} m_k, \text{ and } \Sigma = \frac{1}{K} \sum_{k=1}^{K} (\Sigma_X^{1/2} \Sigma_k \Sigma_X^{1/2})^{1/2}. \] (15)
Note (15) provides \(\Sigma\) in an implicit form, and its computation is a fixed point iteration of a fast algorithm [22]:
\[ \Sigma_{n+1} = \Sigma_n^{-1/2} \left( \frac{1}{K} \sum_{k=1}^{K} (\Sigma_X^{1/2} \Sigma_k \Sigma_X^{1/2})^{1/2} \right)^2 \Sigma_n^{-1/2}. \] (16)

C. Expectation Distance Formulation

While OMT-based distance measure is novel, it ignores the true correlation information: The minimization in (12) is achieved when the two given marginals are most correlated. Recognizing this limitation of \(W_2\) distance (that it is defined for pairwise marginal distributions ignoring their true correlation information), we hereby propose a new and more general distance measure ignoring their true correlation:

\[ p := ||x - y||^2 = 0 \iff E[p] = 0 \iff d_{X,Y}^2 = 0. \]

Triangle Inequality (\(d_{X,Z} \leq d_{X,Y} + d_{Y,Z}\)):

By Minkowski inequality in \(L^2\) spaces:
\[ d_{X,Z} \left[ E[||X - Z||^2]^\frac{1}{2} \right] \leq \left[ E[||X - Y||^2 + ||Y - Z||^2] \right] \frac{1}{2} \leq \left[ E[||Y - Z||^2] \right] \frac{1}{2} = d_{Y,Z} + d_{X,Y}. \]
This concludes the proof that the ED proposed in (17) is indeed a distance measure.

1) Cluster-center: Under the ED measure, the cluster-center in case of \(K\)-means for a cluster \(C\) is given by,
\[ \arg\inf_{\mu \in C} \sum_{\mu \in C} E[||\mu' - \mu||^2], \] (18)
where the optimization is with respect to all sets of joint distributions whose marginals satisfy the condition as stated in (18). It can then be seen that the above cost function is the same as that of \(W_2\)-based distance in (19), and hence the resulting cluster-center in the case of ED-distance for \(K\)-means is again the Barycenter \(\frac{1}{\pi} \sum_{\mu \in C} \mu\).

Similar to \(W_2\), in the case of \(K\)-medoids, a cluster-center is chosen to be one of the data points, and so their joint distribution is already estimated from the data:
\[ \arg\min_{\mu \in C} \sum_{\mu \in C} E[||\mu' - \mu||^2]. \] (19)

Next, we discuss how to compute its value for the case of Gaussian distributions.

2) Expectation Distance for Gaussian distributions: Given two random Gaussian distributions, \(\mu_X = \mathcal{N}(m_X, \Sigma_X)\) and \(\mu_Y = \mathcal{N}(m_Y, \Sigma_Y)\), from (11) their ED can be represented by:
\[ d_{X,Y}^2 = E[||X - Y||^2] = tr(\Sigma_X + \Sigma_Y - 2\Sigma_{XY}) + ||m_X - m_Y||^2. \] (20)
It can be noted that in case the correlation \(\Sigma_{XY}\) of the two random variables is the same as the one given in (13), the ED distance coincides with the \(W_2\) distance. However, in general, ED is higher: To attain the minimization of (12), which is a decreasing function of \(\Sigma_{XY}\), its largest possible value gets picked, but in reality, \(\Sigma_{XY}\) may be smaller, leading to ED being larger than \(W_2\).

3) Joint Distribution with cluster-center: For \(K\)-means, a Barycenter (namely, the center of mass of a cluster) serves as the cluster center. As per (2), which provides a formula for the Barycenter, it is independent of the distance measure used, and so it is the same for both \(W_2\) and ED distance measures. In order to measure the distance of a distribution \(x\) to a cluster-center \(c\) (which is a Barycenter in case of \(K\)-means), a task is to find the joint distribution of \(x\) and \(c\), which for \(K\)-means is the center of mass of a cluster of distributions, say, \(x_1, x_2, \ldots, x_m\). From (20), for the computation of ED between \(x\) and \(c\), it suffices to compute the joint covariance.
of $x$ and $c$, which we obtain by noting the following linear identity:

$$\text{Cov}(x, c) = \text{Cov}(x, \frac{x_1 + x_2 + \ldots + x_m}{m})$$

$$= \frac{1}{m} \left\{ \text{Cov}(x, x_1) + \text{Cov}(x, x_2) + \ldots + \text{Cov}(x, x_m) \right\}.$$  

(21)

D. $W_2$nd ED distances-based noise-robust clustering

Here the classical $K$-means and $K$-medoids-based clustering methods have been adapted by performing the clustering over the data distributions (as opposed to raw data) and then assigning the data to the cluster of its distribution. The distance measures considered in clustering over the data distributions are the above-mentioned $W_2$ and ED distances. The corresponding $K$-means clustering algorithm is presented in Algorithms 1 and 2 and the corresponding $K$-medoids clustering algorithm is presented in Algorithms 3 and 4. It should be noted that for $K$-means clustering, the cluster-center is the Barycenter, and by the definition of Barycenter (2), it does not involve any distance measure, meaning that the Barycenter is the same for both $W_2$ and ED distance measures in the case of $K$-means. The situation is not the same in the case of $K$-medoids, and the choice of distance, $W_2$ versus ED, matters in the determination of cluster-center. In both $K$-means and $K$-medoids, the distances between data points and cluster-centers are measured differently under $W_2$ vs. ED, affecting the clustering results in the $W_2$ vs. ED cases. This is also made evident from our implementation results presented in the next section.

Each algorithm starts with an initial guess of $K$ cluster-centers, and iteratively assigns data to the nearest cluster-center, and then recomputes the cluster-centers until convergence is reached.

Algorithm 1 Distribution-based $K$-means using $W_2$

1: Choose $K$ initial cluster-centers $c_1, c_2, \ldots, c_K$ for the given set of $N$ data, $X = \{x_1, x_2, \ldots, x_N\}$. 
2: for $i = 1$ to $N$ (=total number of data points) do
3:  Solve
4:  Assign $x_i$ to cluster $k_i$
5: end for
6: for $k = 1$ to $K$ (=total number of clusters) do
7:  Update center $c_k = \text{Barycenter}(X_k)$
8: end for
9: Repeat steps 2 to 8 using new $c_k$’s until convergence.

Algorithm 2 Distribution-based $K$-means using ED

Same as Algorithm 1, with the following changed step 3:
3:  $k_i = \arg \left\{ \min_{1 \leq k \leq K} d^2_{x_i, c_k} \right\}$.

III. RESULTS AND DISCUSSION

The distance-based noise-robust algorithms have been formulated to cluster both synthetic data and noisy real-world data.

A. Result 1: Synthetic data

This first result is designed to show that the distribution-based clustering algorithms are better equipped for noisy data clustering when compared to the classical algorithms. For this, we consider synthetic data of Gaussian distributed randomly generated 2D numbers of size $1500 \times 2$, where the data:

$$X \sim \left\{ \begin{array}{l}
\frac{3}{4} \times \text{randn}(500, 1) + 1 \\
\frac{3}{4} \times \text{randn}(500, 1) - 1
\end{array} \right\},$$

is to be grouped into 3 clusters. The marginal and joint distributions were computed using 20 samples each, and hence the distribution data is a 2-dimensional data of size $1500/20=75$. Results are shown in Figs. 1 and 2.

From the summary results of Table 1 the distribution-based $K$-means and $K$-medoids versions are 96.47%, 100%, and 100% respectively, whereas the accuracies of the corresponding $K$-medoids versions are 96.53%, 100%, and 100% respectively.

As observed in Table 1 the two distribution-based $K$-means ($W_2$ vs. ED) have similar means and covariances. This is
B. Result 2: Synthetic data with unbalanced cluster size

The clusters formed by classical $K$-means and $K$-medoids clustering depend on the cluster centroids. If the centroids are close to one another, then the resulting clusters may be skewed. If the original clusters have an unbalanced length of data points, then by choosing the initial cluster-centers randomly, there is a high probability that one would choose the initial cluster-centers from the same cluster. This is a common problem encountered in partition-based clustering. To illustrate the surrounding issues and show that our algorithm is robust enough to cluster even unbalanced sized data, we consider synthetic data of Gaussian distributed random numbers of size $3000 \times 2$:

$$X \sim \begin{bmatrix} \text{randn}(2000, 1) & 4 \times \text{randn}(2000, 1) - 2 \\ \text{randn}(500, 1) - 8 & 2 \times \text{randn}(500, 1) - 1 \\ \text{randn}(500, 1) + 8 & 2 \times \text{randn}(500, 1) - 1 \end{bmatrix},$$

where $X$ is to be grouped into 3 clusters. The marginal and joint distributions were similarly computed over 20 samples each, and hence the distribution data is a 2-dimensional data of size $3000/20=150$. Results are shown in Figs. 3 and 4.

From the summary results of Table I, the distribution-based $K$-means and $K$-medoids under both distance measures outperform the corresponding classical versions: The accuracies of classical $K$-means, $W_2$ $K$-means, and ED $K$-means are 72.4%, 100%, and 100% respectively, whereas the accuracies of the corresponding $K$-medoids versions are 73.3%, 100%, and 100% respectively. There is a dramatic improvement over the classical clustering due to the known fact that they do not work well with unbalanced sized data [24].

Table II: Table of accuracy of result 2

| Algorithm       | Accuracy(%) | Centers/Cluster-center indices |
|-----------------|-------------|--------------------------------|
| Classical $K$-means | 72.4        |                                |
| $W_2$ $K$-means  | 100         | means: $[-0.0391 \ 1.9316]^T$  |
|                 |             | $[-7.9458 \ 0.9100]^T$         |
|                 |             | $[7.9681 \ -0.8576]^T$         |
| ED $K$-means    | 100         | means: $[-0.0391 \ 1.9316]^T$  |
|                 |             | $[-7.9458 \ 0.9100]^T$         |
|                 |             | $[7.9681 \ -0.8576]^T$         |
| Classical $K$-medoids | 73.3        |                                |
| $W_2$ $K$-medoids | 100         | Center indices: $(69, 144, 119)$|
| ED $K$-medoids   | 100         | Center indices: $(132, 117, 55)$|
A daily weather data of 8-year duration (2011-2018) was obtained from Carbondale station. We extracted two major weather variables: Maximum daily Temperature ($^\circ$C) and Vapor pressure (kPa). For easy computation of data distributions, we considered the first 28 days of each month, and so the size of data is $28 \times 12 \times 8 = 2688$ number of 2-dimensional entries. The goal was to cluster the data into 4 clusters corresponding to the 4 seasons, in accordance to the 4 meteorological seasons in USA:

- Spring: 03/01 - 05/31;
- Summer: 06/01 - 08/31;
- Fall: 09/01 - 11/30;
- Winter: 12/01 - 02/28.

Accordingly, the marginal and joint distributions were computed seasonally, and hence in the span of 8 years, we obtained a total of 32 seasons of marginal data distributions and $32 \times 32$ joint distributions. Each distribution mean is 2-dimensional, and each joint distribution covariance matrix is of size $2 \times 2$. Results are shown in figs (3) and (4).

From the summary results of Table III, the distribution-based $K$-means and $K$-medoids under both distance measures strikingly outperform the corresponding classical versions: The accuracies of classical $K$-means, $W_2$ $K$-means, and ED $K$-means are 49.52%, 93.75%, and 100% respectively, whereas the accuracies of the corresponding $K$-medoids versions are 49.26%, 93.75%, and 100% respectively. Also, in both $K$-means and $K$-medoids, the ED-based distance measurement offers higher accuracy than the $W_2$ based ones.

| Algorithm     | Accuracy(%) | Centers/Cluster-center indices |
|---------------|-------------|--------------------------------|
| Classical $K$-means | 49.52 | [Center: (32, 27, 13, 2)] |
| $W_2$ $K$-means    | 93.75 | [Center: (7, 22, 20, 29)] |
| ED $K$-means      | 100  | [Center: (32, 27, 13, 2)] |
| Classical $K$-medoids | 49.26 | [Center: (32, 27, 13, 2)] |
| $W_2$ $K$-medoids | 93.75 | [Center: (7, 22, 20, 29)] |
| ED $K$-medoids    | 100  | [Center: (7, 22, 20, 29)] |

As noted in Table III, the two distribution-based $K$-means ($W_2$ vs. ED) have similar means and covariances for the first two clusters. This is as a result of them having the same data points in the two clusters. However, the other two clusters show that ED performs better over $W_2$, which may have been
both clusters corresponding real-world weather data by efficiently extracting and using other. Again ED offers higher accuracy than means are independent of the distance measure used, the same based distribution. We also observed that the first and then assigned each raw data to the cluster of its distribution. For the case of distribution-based clustering to over the data distributions (rather the raw data), types of measures: and for this, measured distances among distributions using two that while the cluster centers of the distribution-based on the pairwise marginal distributions, ignoring the true correlation information. In contrast, the proposed ED overcomes this limitation by factoring in the correlation information and, in the process, yields more noise-robust results. We also noted that while the cluster centers of the distribution-based K-means are independent of the distance measure used, the same is not true of K-medoids. We implemented these noise-robust distance-based algorithms and applied them to cluster noisy real-world weather data by efficiently extracting and using underlying uncertainty information (means and variances). The results on weather data showed striking improvement in performance for W2 and ED distance-based K-means and K-medoids, where higher accuracy was observed for ED in both K-means and K-medoids: The accuracies of classical K-means, W2 K-means, and ED, K-means were 49.52%, 93.75%, and 100%, respectively, whereas the accuracies of the corresponding K-medoids versions were 49.26%, 93.75%, and influenced by the low correlation between the corresponding distributions being clustered. For the case of distribution-based K-medoids, the cluster-center indices for W2 and ED-based distances are listed in Table III and those differ from each other. Again ED offers higher accuracy than W2.

IV. CONCLUSION

The paper extended the classical K-means and K-medoids clustering to over the data distributions (rather the raw data), and for this, measured distances among distributions using two types of measures: W2 and ED. The presented distribution-based K-means and K-medoids cluster the data distributions first and then assigned each raw data to the cluster of its distribution. We also observed that the W2 distance only depends on the pairwise marginal distributions, ignoring the true correlation information. In contrast, the proposed ED overcomes this limitation by factoring in the correlation information and, in the process, yields more noise-robust results. We also noted that while the cluster centers of the distribution-based K-means are independent of the distance measure used, the same is not true of K-medoids. We implemented these noise-robust distance-based algorithms and applied them to cluster noisy real-world weather data by efficiently extracting and using underlying uncertainty information (means and variances). The results on weather data showed striking improvement in performance for W2 and ED distance-based K-means and K-medoids, where higher accuracy was observed for ED in both K-means and K-medoids: The accuracies of classical K-means, W2 K-means, and ED, K-means were 49.52%, 93.75%, and 100%, respectively, whereas the accuracies of the corresponding K-medoids versions were 49.26%, 93.75%, and 100% respectively. Clearly, in both K-means and K-medoids, the proposed ED-based measurement offered higher accuracy than the W2 based distance.

REFERENCES

[1] M. Chau, R. Cheng, and B. Kao, “Uncertain data mining: A new research direction,” 2005.
[2] C. Aggarwal and P. Yu, “A survey of uncertain data algorithms and applications,” Knowledge and Data Engineering, IEEE Transactions on, vol. 21, pp. 609 – 623, 06 2009.
[3] C. C. Aggarwal, Managing and Mining Uncertain Data, 2009, vol. 35.
[4] B. Kao, S. D. Lee, F. K. Lee, D. W. Cheung, and W.-S. Ho, “Clustering uncertain data using voronoi diagrams and r-tree index,” IEEE Transactions on Knowledge and Data Engineering, vol. 22, no. 9, pp. 1219–1233, 2010.
[5] B. Jiang, J. Pei, Y. Tao, and X. Lin, “Clustering uncertain data based on probability distribution similarity,” IEEE Transactions on Knowledge and Data Engineering, vol. 25, no. 4, pp. 751–763, 2013.
[6] R. Cheng, D. V. Kalashnikov, and S. Prabhakar, “Evaluating probabilistic queries over imprecise data,” in Proceedings of the 2003 ACM SIGMOD International Conference on Management of Data, ser. SIGMOD ’03. New York, NY, USA: Association for Computing Machinery, 2003, p. 551–562. [Online]. Available: https://doi.org/10.1145/872575.872823
[7] J. Pei, B. Jiang, X. Lin, and Y. Yuan, “Probabilistic skylines on uncertain data,” in VLDB, 2007.
[8] Y. Tao, R. Cheng, X. Xiao, W. K. Ngai, B. Kao, and S. Prabhakar, “Indexing multi-dimensional uncertain data with arbitrary probability density functions,” in Proceedings of the 31st International Conference on Very Large Data Bases, ser. VLDB ’05. VLDB Endowment, 2005, p. 922–933.
[9] T. A. Gullo F., Ponti G., Clustering Uncertain Data Via K-Medoids. In: Greco S., Lukasiewicz T. (eds) Scalable Uncertainty Management,SUM 2008. Lecture Notes in Computer Science. Springer, Berlin, Heidelberg., 2008, vol. 5291. [Online]. Available: https://doi.org/10.1007/978-3-540-87901-010
[10] Y. Peng, Q. Luo, and X. Peng, “UCK-means: A customized k-means for clustering uncertain measurement data,” 2011 Eighth International Conference on Fuzzy Systems and Knowledge Discovery (FSKD), 2011.
[11] C. C. Aggarwal, “On density based transforms for uncertain data mining,” in 2007 IEEE 23rd international conference on data engineering. IEEE, 2007, pp. 866–875.

[12] W. K. Ngai, B. Kao, C. Chui, R. Cheng, M. Chau, and K. Y. Yip, “Efficient clustering of uncertain data,” Sixth International Conference on Data Mining (ICDM’06), pp. 436–445, 2006.

[13] S. D. Lee, B. Kao, and R. Cheng, “Reducing uk-means to k-means,” in Seventh IEEE International Conference on Data Mining Workshops (ICDMW 2007), 2007, pp. 483–488.

[14] G. Cormode and A. McGregor, “Approximation algorithms for clustering uncertain data,” in Proceedings of the Twenty-Seventh ACM SIGMOD-SIGACT-SIGART Symposium on Principles of Database Systems, ser. PODS ‘08. New York, NY, USA: Association for Computing Machinery, 2008, p. 191–200. [Online]. Available: https://doi.org/10.1145/1376916.1376944

[15] M. Ester, H.-P. Kriegel, J. Sander, and X. Xu, “A density-based algorithm for discovering clusters in large spatial databases with noise,” in Proceedings of the Second International Conference on Knowledge Discovery and Data Mining, ser. KDD’96. AAAI Press, 1996, p. 226–231.

[16] M. Ankerst, M. M. Breunig, H.-P. Kriegel, and J. Sander, “Optics: Ordering points to identify the clustering structure,” in Proceedings of the 1999 ACM SIGMOD International Conference on Management of Data, ser. SIGMOD ’99. New York, NY, USA: Association for Computing Machinery, 1999, p. 49–60. [Online]. Available: https://doi.org/10.1145/304182.304187

[17] H.-P. Kriegel and M. Pfeifle, “Density-based clustering of uncertain data,” in Proceedings of the Eleventh ACM SIGKDD International Conference on Knowledge Discovery in Data Mining, ser. KDD ’05. New York, NY, USA: Association for Computing Machinery, 2005, p. 672–677. [Online]. Available: https://doi.org/10.1145/1081870.1081955

[18] ——, “Hierarchical density-based clustering of uncertain data,” in Fifth IEEE International Conference on Data Mining (ICDM’05), 2005, pp. 4 pp.–.

[19] J. Ye, P. Wu, J. Z. Wang, and J. Li, “Fast discrete distribution clustering using wasserstein barycenter with sparse support,” IEEE Transactions on Signal Processing, 2017.

[20] G. Domazakis, D. Drivaliaris, S. Koukoulas, G. I. Papayiannis, A. E. Tsekrekos, and A. N. Yannacopoulos, “Clustering measure-valued data with wasserstein barycenters,” 2019.

[21] M. Chau, R. Cheng, B. Kao, and J. Ng, “Uncertain data mining: An example in clustering location data,” in Advances in Knowledge Discovery and Data Mining, W.-K. Ng, M. Kitsuregawa, J. Li, and K. Chang, Eds. Berlin, Heidelberg: Springer Berlin Heidelberg, 2006, pp. 199–204.

[22] Y. Chen, T. T. Georgiou, and A. Tannenbaum, “Optimal transport for gaussian mixture models,” IEEE Access, vol. 7, pp. 6269–6278, 2019.

[23] S. Kolouri, S. R. Park, M. Thorpe, D. Slepcev, and G. K. Rohde, “Optimal mass transport: Signal processing and machine-learning applications,” IEEE Signal Processing Magazine, 2017.

[24] J. Liang, L. Bai, C. Dang, and F. Cao, “The \( f \)-formula for \( \text{f-formula} = \text{f-formula} \)-type algorithms versus imbalanced data distributions,” IEEE Transactions on Fuzzy Systems, vol. 20, no. 4, pp. 728–745, 2012.