Clustering with Missing Features: A Penalized Dissimilarity Measure based approach

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Abstract

Many real-world clustering problems are plagued by incomplete data characterized by missing or absent features for some or all of the data instances. Traditional clustering methods cannot be directly applied to such data without preprocessing by imputation or marginalization techniques. In this article, we put forth the concept of Penalized Dissimilarity Measures which estimate the actual distance between two data points (the distance between them if they were to be fully observed) by adding a penalty to the distance due to the observed features common to both the instances. We then propose such a dissimilarity measure called the Feature Weighted Penalty based Dissimilarity (FWPD) measure. Using the proposed dissimilarity measure, we also modify the traditional k-means clustering algorithm and the standard hierarchical agglomerative clustering techniques so as to make them directly applicable to datasets with missing features. We present time complexity analyses for these new techniques and also present a detailed analysis showing that the new FWPD based k-means algorithm converges to a local optimum within a finite number of iterations. We have also conducted extensive experiments on various benchmark datasets showing that the proposed clustering techniques have generally better results compared to some of the popular imputation methods which are commonly used to handle such incomplete data. We have appended a possible extension of the proposed dissimilarity measure to the case of absent features (where the unobserved features are known to be non-existent).

Keywords: Missing Features, Penalized Dissimilarity Measure, k-means, Hierarchical Agglomerative Clustering, Absent Features
1. Introduction

1.1. Overview

Clustering is a fundamental problem in data analysis that is concerned with dividing a given dataset into useful groups (called clusters) according to their relative similarity. Clustering algorithms attempt to partition a set of data instances (characterised by some features), into different clusters such that member instances of any given cluster are akin to each other and are different from the members of the other clusters. Greater the similarity within a group and the dissimilarity between groups, better is the clustering obtained by a suitable algorithm.

Clustering techniques are of extensive use and are hence being constantly investigated in statistics, machine learning, and pattern recognition. Clustering algorithms find applications in various fields such as economics, marketing, electronic design, space research, etc. For example, clustering has been used to group related documents for web browsing, by banks to cluster the previous transactions of clients to identify suspicious (possibly fraudulent) behaviour, for formulating effective marketing strategies by clustering customers with similar behaviour, in earthquake studies for identifying dangerous zones based on previous epicentre locations, and so on. However, when we analyze such real-world data, we may encounter incomplete data where some features of some of the data instances are missing. For example, web documents may have some expired hyper-links. Such missingness may be due to a variety of reasons such as data input errors, inaccurate measurement, equipment malfunction or limitations, and measurement noise or data corruption, etc. This is known as unstructured missingness \[1, 2\]. Alternatively, not all the features may be defined for all the data instances in the dataset. This is termed as structural missingness or absence of features \[3\]. For example, credit-card details may not be defined for non-credit clients of a bank.

Missing features have always been a challenge for researchers because traditional learning methods (which assume all data instances to be fully observed, i.e. all the features are observed) cannot be directly applied to such incomplete data, without suitable preprocessing. When the rate of missingness is low, such as \(1 - 5\%\), the data instances with missing values is ignored. This approach is known as marginalization. Marginalization cannot be applied to data having \(5 - 15\%\) missing values, as it may lead to the loss of a sizable amount of information. Therefore, sophisticated methods are required to fill in the vacancies in the data, so that traditional learning methods can be applied subsequently. This approach of filling in the missing values is called imputation. Inferences drawn from data having more than \(15\%\) missingness may be severely warped, despite the use of such sophisticated imputation methods \[4\].
1.2. Literature

The initial models for feature missingness are due to Rubin and Little [2] [5]. They proposed a three-fold classification of missing data mechanisms, viz. Missing Completely At Random (MCAR), Missing At Random (MAR), and Missing Not At Random (MNAR). MCAR refers to the case where missingness is entirely haphazard, i.e. the likelihood of a feature being unobserved for a certain data instance depends neither on the observed nor on the unobserved characteristics of the instance. For example, in an annual income survey, a citizen is unable to participate, due to unrelated reasons such as traffic or schedule problems. MAR eludes to the cases where the missingness is conditional to the observed features of an instance, but is independent of the unobserved features. Suppose, college-goers are less likely to report their income than office-goers. But, whether a college-goer will report his/her income is independent of the actual income. MNAR is characterised by the dependence of the missingness on the unobserved features. For example, people who earn less are less likely to report their incomes in the annual income survey. Schafer & Graham [6] and Zhang et al. [7] have observed that MCAR is a special case of MAR and that MNAR can also be converted to MAR by appending a sufficient number of additional features. Therefore, most learning techniques are based on the validity of the MAR assumption.

A lot of research on the problem of learning with missing/absent features has been conducted over the past few decades, mostly focussing on imputation methods. Several works such as [5] and [8] provide elaborate theories and analyses of missing data. Common imputation methods [9] involve filling the missing features of data instances with zeros (Zero Imputation (ZI)), or the means of the corresponding features over the entire dataset (Mean Imputation (MI)). Class Mean Imputation or Concept Mean Imputation (CMI) is a slight modification of MI that involves filling the missing features with the average of all observations having the same label as the instance being filled. Yet another common imputation method is k-Nearest Neighbour Imputation (kNNI) [10], where the missing features of a data instance are filled in by the means of corresponding features over its k-Nearest Neighbours (kNN), on the observed subspace. Grzymala-Busse & Hu [11] suggested different approaches for filling in the missing feature values, viz selecting the most common feature value, selecting the most common value of the feature within the same class or concept, C4.5 based imputation, assigning all possible values of the feature, assigning all possible values of the feature restricted to the given concept or class, marginalization, treating missing attribute values as special values, event-covering method, etc.

Rubin’s book [12] on Multiple Imputation (MtI) proposes a technique where the missing values are imputed by a typically small (e.g. 5-10) number of simulated versions, depending on the percentage of missing data. This method of repeated imputation incorporates the uncertainty inherent in imputation. Techniques such as Markov Chain Monte Carlo (MCMC) [13] (which simulates random draws from nonstandard distributions via Markov chains) have been used for MtI by making a few independent
estimates of the missing data from a predictive distribution; and these estimates are then used for MtI ([14], [15]). However, imputation methods may introduce noise and create more problems than they solve, as documented by Little & Rubin [5] and others [16, 17, 18].

Model-based methods that make use of the inter-relationships among the features to handle the missing data have shown vast improvements over traditional imputation approaches [19, 20, 21]. These procedures are somewhat more efficient than MtI because they often achieve better estimates of the missing feature values. Generally, in incomplete datasets, Maximum Likelihood Estimation (MLE) is used when we can maximize the likelihood function. The likelihoods are separately calculated for cases with unobserved features and for cases with complete data on all features. Then, these two likelihoods are maximized together to obtain the estimates. Dempster & Rubin [18] proposed the use of an iterative solution, based on the Expectation Maximization (EM) algorithm, when closed form solutions to the maximization of likelihoods are not possible. Some more sophisticated techniques have been developed, especially by the bioinformatics community, which impute the missing values by exploiting the correlations between data. Troyanskaya et al. [22] proposed a weighted variant of kNNI and also put forth the Singular Value Decomposition based Imputation (SVDI) technique, which performs regression based estimation of the missing values using the k most significant Eigenvectors of the dataset. Two variants of the Least Squares Imputation (LSI) technique were proposed by Bo et al. [23]. Sehgal et al. [24] further combined LSI with Non-Negative LSI (NNLSI) in the Collateral Missing Value Estimation (CMVE) technique. These methods have also been shown to vastly improve the results [25, 26].

However, model-based approaches are often computationally expensive. Moreover, most imputation methods assume that the response mechanism underlying the missingness is ignorable. When data are MCAR or MAR, it is said that the response mechanism is ignorable. In such cases, the reasons for missing data may be ignored and simpler models can be used for missing data analysis. Heitjan & Basu [27] provided a thorough discussion of this topic. Therefore, most imputation techniques make sense only when the features are known to exist and to be missing at random (MAR/MCAR). On the other hand, MNAR has non-ignorable response mechanism because the mechanism governing the missingness of data itself has to be modeled to deal with the missing data. Hence, other methods have to be developed to tackle incomplete data due to MNAR [28]. Also, as observed earlier, imputation may often lead to introduction of noise and uncertainty in the data. In the analysis of incomplete data, the mechanism and extent of missingness, both are crucial in determining the methods to process them. Therefore, it also makes little sense to use imputation to handle structural missingness (where the unobserved features are known to be undefined).

In light of the observations made in the preceding paragraph, some learning methods avoid the inexact methods of imputation (as well as marginalization) altogether, while dealing with missingness.
Krause & Polikar [29] proposed a modification of the Learn++ incremental learning algorithm which can work around the need for imputation by using an ensemble of multiple classifiers learned on random subspaces of the dataset. Juszczak & Duin [30] trained single class classifiers on each of the features (or combination thereof) so that an inference about the class to which a particular data instance belongs can be drawn even when some of the features are missing, by combining the individual inferences drawn by each of the classifiers pertaining to the observed features. Random subspace learning was also used by Nanni et al. [31] and compared with other approaches such as MI, MtI, etc. Chechik et al. [3] used the geometrical insight of max-margin classification to formulate an objective function which was optimized to directly classify the incomplete data. This was extended to the max-margin regression case for software effort prediction with absent features in [7]. Hathaway & Bezdek [32] used the Partial Distance Strategy (PDS) of [10] to extend the Fuzzy C-Means (FCM) clustering algorithm to cases with missing features. PDS scales up observed distance, i.e. the distance between two data instances in their common observed subspace (the subspace consisting of the observed features common to both data instances) by the ratio of the total number of features (observed as well as unobserved) and the number of common observed features between them to obtain an estimate of their distance in the fully observed space. However, the PDS may not always provide a good estimate of the actual distance as the observed distance between two instances may be unrelated to the distance between them in the unobserved subspace. Wagstaff et al. [33, 34] suggested a k-means algorithm with Soft Constraints (KSC) where soft constraints determined by fully observed objects are introduced to help with the grouping of instances with missing features. It was applied as an alternative to imputation or marginalization techniques for astronomical data from the Sloan Digital Sky Survey where missing values are also of significance and should not be filled in with imputations. Himmelspach & Conrad [35] provided a good review of partitional clustering techniques for incomplete datasets, which mentions some other techniques that do not resort to imputation.

1.3. Motivation

One possible way to adapt supervised as well as unsupervised learning methods to problems with missingness is to modify the distance or dissimilarity measure underlying the learning method, so that the modified dissimilarity measure uses the common observed features to provide approximations of the distances between the data instances if they were to be fully observed. PDS is one such measure. Such approaches neither require marginalization nor imputation, while possibly yielding better results than either of the two. Let us look at an example. Let $X_{full} = \{x_1 = (1,5), x_2 = (2,3), x_3 = (3,6)\}$ be a dataset consisting of three points in $\mathbb{R}^2$. Then, the distances $d_E(x_1, x_2)$ and $d_E(x_1, x_3)$ (where $d_E(x_i, x_j)$ denotes the Euclidean distance between the fully observed points $x_i$ and $x_j$ in $X_{full}$) are $d_E(x_1, x_2) = \sqrt{5}$ and $d_E(x_1, x_3) = \sqrt{5}$, respectively. Now, let the 1st coordinate of the point $(1,5)$
be unobserved. Then, the resulting dataset, on which learning must be undertaken, is \( X = \{ \mathbf{x}'_1 = (\ast, 5), \mathbf{x}_2 = (2, 3), \mathbf{x}_3 = (3, 6) \} \), where ‘\( \ast \)’ denotes an unobserved value. Notice that this is a case of unstructured missingness (because the unobserved value is known to exist), as opposed to the structural missingness of [3]. Then the filled in datasets \( X_{ZI}, X_{MI}, \) and \( X_{1NNI} \) obtained respectively using ZI, MI and 1NNI (kNNI with \( k = 1 \)) are

\[
\begin{align*}
X_{ZI} &= \{ \hat{x}_1 = (0, 5), \mathbf{x}_2 = (2, 3), \mathbf{x}_3 = (3, 6) \}, \\
X_{MI} &= \{ \hat{x}_1 = (2.5, 5), \mathbf{x}_2 = (2, 3), \mathbf{x}_3 = (3, 6) \}, \\
\text{and } X_{1NNI} &= \{ \hat{x}_1 = (3, 5), \mathbf{x}_2 = (2, 3), \mathbf{x}_3 = (3, 6) \},
\end{align*}
\]

where \( \hat{x}_1 \) denotes an estimate of \( \mathbf{x}_1 \). If PDS is used to estimate the corresponding distances in \( X \), then the estimated distance \( d_{PDS}(\mathbf{x}_1, \mathbf{x}_i) \) between \( \mathbf{x}'_1 \) and some other instance \( \mathbf{x}_i \in X \) is obtained by

\[
d_{PDS}(\mathbf{x}_1, \mathbf{x}_i) = \sqrt{\frac{2}{1} (x_{1,2} - x_{i,2})^2},
\]

where \( x_{1,2} \) and \( x_{i,2} \) respectively denote the 2nd features of \( \mathbf{x}'_1 \) and \( \mathbf{x}_i \), and 2 is the numerator of the multiplying factor due to the fact that \( \mathbf{x}_1 \in \mathbb{R}^2 \) and 1 is the denominator owing to the fact that only the 2nd feature is observed for both \( \mathbf{x}'_1 \) and \( \mathbf{x}_i \). Then, we get

\[
d_{PDS}(\mathbf{x}_1, \mathbf{x}_2) = \sqrt{\frac{2}{1} (5 - 3)^2} = \sqrt{8},
\]

and

\[
d_{PDS}(\mathbf{x}_1, \mathbf{x}_3) = \sqrt{\frac{2}{1} (5 - 6)^2} = \sqrt{2}.
\]

The erroneous estimates obtained by PDS are due to the fact that the distance in the common observed subspace does not reflect the distance in the unobserved subspace. This is the principal drawback of the PDS method, as discussed earlier. Since the observed distance between two data instances is essentially a lower bound on the Euclidean distance between them (if they were to be fully observed), adding a suitable penalty to this lower bound can yield a reasonable approximation of the actual distance. This new approach, which we call the Penalized Dissimilarity Measure (PDM), may be able to overcome the drawback which plagues PDS. Let the penalty between \( \mathbf{x}'_1 \) and \( \mathbf{x}_i \) be given by the ratio of the number of features which are unobserved for at least one of the two data instances and the total number of features in the entire dataset. Then, the dissimilarity \( \delta'(\mathbf{x}_1, \mathbf{x}_i) \) between \( \mathbf{x}'_1 \) and some other \( \mathbf{x}_i \in X \) is

\[
\delta'(\mathbf{x}_1, \mathbf{x}_i) = \sqrt{(x_{1,2} - x_{i,2})^2 + \frac{1}{2}},
\]

where the 1 in the numerator of the penalty term is due to the fact that the 1st feature of \( \mathbf{x}'_1 \) is unobserved. Therefore, the dissimilarities \( \delta'(\mathbf{x}_1, \mathbf{x}_2) \) and \( \delta'(\mathbf{x}_1, \mathbf{x}_3) \) are

\[
\delta'(\mathbf{x}_1, \mathbf{x}_2) = \sqrt{(5 - 3)^2 + \frac{1}{2}} = 2.5,
\]

and

\[
\delta'(\mathbf{x}_1, \mathbf{x}_3) = \sqrt{(5 - 6)^2 + \frac{1}{2}} = 1.5.
\]
The situation is illustrated in Figure 1. The reader should note that while the points estimated using ZI, MI and 1NNI exist in the same 2-D Cartesian space to which $X_{full}$ is native, the points estimated by both PDS and PDM exist in their individual abstract spaces (likely distinct from the native 2-D space). However, for the sake of easy comparison, we have illustrated all the estimates together by superimposing both these abstract spaces on the native 2-D space so as to coincide at the points $x_2$ and $x_3$. It can be seen that the approach based on the PDM does not suffer from the drawback of PDS and is better able to preserve the relationship between the points. Moreover, such a PDM can also be easily applied to the case of absent features, by slightly modifying the penalty term (see Appendix A). This knowledge motivates us to propose a PDM which can be used to adapt traditional learning methods to problems with missing/absent features.

1.4. Contribution

In this study, we have proposed a PDM called the Feature Weighted Penalty based Dissimilarity (FWPD) measure and used it to adapt common clustering algorithms to the missing data problem. The FWPD between two data instances is a weighted sum of two terms; the first term being the observed distance between the instances and the second being a penalty term. The penalty term is a sum of the penalties corresponding to each of the features which are missing from at least one of
the data instances; each penalty being directly proportional to the probability of its corresponding feature being observed. The proposed weighting scheme is meant to limit the impact of each feature as per its availability in the observed dataset. This novel dissimilarity measure is incorporated into both partitional as well as Hierarchical Agglomerative Clustering (HAC) algorithms over data suffering from unstructured missingness. We have formulated the k-means clustering problem for datasets with missing features based on the proposed FWPD and developed an algorithm to solve the new formulation. We have proved that the proposed algorithm is guaranteed to converge to a locally optimal solution of the modified k-means optimization problem formulated with the FWPD measure. We have also proposed Single Linkage (SL), Average Linkage (AL), and Complete Linkage (CL) based HAC methods for datasets plagued by missingness, based on the proposed FWPD. Experiments have been conducted on diverse datasets and the results have been compared with the popularly used imputation techniques. The comparative results indicate that our approach generally achieves better performance than the common imputation approaches used to handle incomplete data. Moreover, since this work presents an alternative to imputation and can be useful in scenarios where imputation is not practical (such as structural missingness), we have appended an extension of the proposed FWPD to the case of absent features. The principal difference between missing and absent features lies in the fact that the unobserved features are known to be non-existent in the latter case, unlike the former. Therefore, while it makes sense to add penalties for features which are observed for only one of the data instances (as the very existence of such a feature sets the points apart), it makes little sense to add penalties for features which are undefined for both the data points. This is in contrast to problems with unstructured missingness where a feature missing from both the data instances is known to be defined for both points (which potentially have distinct values of this feature). Hence, it is essential to add penalties for features missing from both points in the case of missing features, but not in the case of absent features. We also show that the FWPD becomes a semimetric in the case of structural missingness.

1.5. Organization

The rest of this paper is organized in the following way. In Section 2, we elaborate on the proposed FWPD measure. The next section (Section 3) presents a formulation of the k-means clustering problem which is directly applicable to datasets with missing features, based on the FWPD discussed in Section 2. This section also puts forth an algorithm to solve the optimization problem posed by this new formulation. The subsequent section (Section 4) covers the SL, AL, and CL based HAC algorithms which are formulated using the FWPD to be directly applicable to incomplete datasets. Experimental results are presented in Section 5 and relevant conclusions are drawn in Section 6. The subsequent Appendix A deals with the extension of the proposed FWPD to the case of absent features (structural
missingness).

2. Feature Weighted Penalty based Dissimilarity Measure for Datasets with Missing Features

Let the dataset \( X \subset \mathbb{R}^m \) consist of \( n \) instances \( x_i \) \( (i \in \{1, 2, \cdots, n\}) \), some of which have missing features. Let \( \gamma_{x_i} \) denote the set of observed features for the data point \( x_i \). Then, the set of all features \( S = \bigcup_{i=1}^n \gamma_{x_i} \) and \( |S| = m \). The set of features which are observed for all data instances in \( X \) is defined as \( \Gamma_{obs} = \bigcap_{i=1}^n \gamma_{x_i} \). \( |\Gamma_{obs}| \) may or may not be non-zero. \( \Gamma_{mis} = S \setminus \Gamma_{obs} \) is the set of features which are unobserved for at least one data point in \( X \).

**Definition 1.** Taking any two data instances \( x_i, x_j \in X \), the observed distance \( d(x_i, x_j) \) between these two points (in the common observed subspace) is defined as

\[
d(x_i, x_j) = \sqrt{\sum_{l \in \gamma_{x_i} \cap \gamma_{x_j}} (x_{i,l} - x_{j,l})^2},
\]

where \( x_{r,s} \) denotes the \( s \)-th feature of the data instance \( x_r \).

**Definition 2.** If both \( x_i \) and \( x_j \) were to be fully observed, the Euclidean distance \( d_E(x_i, x_j) \) between \( x_i \) and \( x_j \) would be defined as

\[
d_E(x_i, x_j) = \sqrt{\sum_{l \in S} (x_{i,l} - x_{j,l})^2}.
\]

Now, since \( (\gamma_{x_i} \cap \gamma_{x_j}) \subseteq S \), and \( (x_{i,l} - x_{j,l})^2 \geq 0 \ \forall \ l \in S \), it follows that

\[
d(x_i, x_j) \leq d_E(x_i, x_j) \ \forall \ x_i, x_j \in X.
\]

Therefore, to compensate for the distance in the unobserved subspace, we add a Feature Weighted Penalty (FWP) \( p(x_i, x_j) \) (defined below) to \( d(x_i, x_j) \).

**Definition 3.** The FWP between \( x_i \) and \( x_j \) is defined as

\[
p(x_i, x_j) = \frac{\sum_{l \in S \setminus (\gamma_{x_i} \cap \gamma_{x_j})} w_l}{\sum_{l' \in S} w_{l'}},
\]

where \( w_s \in (0, n] \) is the number of instances in \( X \) having observed values of the feature \( s \). It should be noted that FWP extracts greater penalty for unobserved occurrences of those features which are observed for a large fraction of the data instances.

Then, the definition of the proposed FWPD follows.
**Definition 4.** The FWPD between $x_i$ and $x_j$ is

$$\delta(x_i, x_j) = (1 - \alpha) \times \frac{d(x_i, x_j)}{d_{\text{max}}} + \alpha \times p(x_i, x_j),$$  \hfill (3)

where $\alpha \in (0, 1)$ is a parameter which determines the relative importance between the two terms and $d_{\text{max}}$ is the maximum observed distance between any two points in $X$ in their respective common observed subspaces.

2.1. Properties of the proposed FWPD

In this subsection, we discuss some of the important properties of the proposed FWPD measure. The following theorem discusses some of the important properties of the proposed FWPD measure and the subsequent discussion is concerned with the triangle inequality with regards to FWPD.

**Theorem 1.** The FWPD measure satisfies the following important properties:

i. $\delta(x_i, x_i) \leq \delta(x_i, x_j) \forall x_i, x_j \in X$,

ii. $\delta(x_i, x_i) = 0$ iff $\gamma_{x_i} = S$, and

iii. $\delta(x_i, x_j) = \delta(x_j, x_i) \forall x_i, x_j \in X$.

**Proof.**

i. From Equations (1) and (3), it follows that

$$\delta(x_i, x_i) = \alpha \times p(x_i, x_i).$$ \hfill (4)

It also follows from Equation (2) that $p(x_i, x_i) \leq p(x_i, x_j) \forall x_i, x_j \in X$. Therefore, $\delta(x_i, x_i) \leq \alpha \times p(x_i, x_j)$. Now, it also follows from Equation (3) that $p(x_i, x_j) \leq \delta(x_i, x_j)$. Hence, we get $\delta(x_i, x_i) \leq \delta(x_i, x_j) \forall x_i, x_j \in X$.

ii. It is easy to see from Equation (4) that $p(x_i, x_i) = 0$ iff $\gamma_{x_i} = S$. Hence, it directly follows from Equation (4) that $\delta(x_i, x_i) = 0$ iff $\gamma_{x_i} = S$.

iii. From Equation (3) we have

$$\delta(x_i, x_j) = (1 - \alpha) \times \frac{d(x_i, x_j)}{d_{\text{max}}} + \alpha \times p(x_i, x_j),$$

and $\delta(x_j, x_i) = (1 - \alpha) \times \frac{d(x_j, x_i)}{d_{\text{max}}} + \alpha \times p(x_j, x_i)$.

However, $d(x_i, x_j) = d(x_j, x_i)$ and $p(x_i, x_j) = p(x_j, x_i) \forall x_i, x_j \in X$ (by definition). Therefore, it can be easily seen that $\delta(x_i, x_j) = \delta(x_j, x_i) \forall x_i, x_j \in X$.

The triangle inequality is an important criterion which, when satisfied, lends some useful properties to the space induced by a dissimilarity measure. Therefore, the conditions under which the FWPD measure satisfies the said criterion are investigated below.
**Definition 5.** For any three data instances \(x_i, x_j, x_k \in X\), the triangle inequality w.r.t. the FWPD measure is defined as

\[
\delta(x_i, x_j) + \delta(x_j, x_k) \geq \delta(x_k, x_i).
\]  

(5)

The following lemmas deal with the conditions under which Inequality (5) will hold.

**Lemma 2.** For any three data points \(x_i, x_j, x_k \in X\), Inequality (5) is satisfied when \((\gamma_S \cap \gamma_{x_i}) = (\gamma_S \cap \gamma_{x_j}) = (\gamma_S \cap \gamma_{x_k})\).

**Proof.** Let \(p_\gamma\) denote the penalty corresponding to the subspace \(\gamma\), i.e. \(p_\gamma = \sum_{l \in S} w_l\). Then, from Equation (5) we have

\[
\delta(x_i, x_j) = (1 - \alpha) \times \frac{d(x_i, x_j)}{d_{\max}} + \alpha \times (p_S(\gamma_{x_i} \cap \gamma_{x_j}))
\]

\[
\delta(x_j, x_k) = (1 - \alpha) \times \frac{d(x_j, x_k)}{d_{\max}} + \alpha \times (p_S(\gamma_{x_j} \cap \gamma_{x_k}))
\]

and \(\delta(x_k, x_i) = (1 - \alpha) \times \frac{d(x_k, x_i)}{d_{\max}} + \alpha \times (p_S(\gamma_{x_k} \cap \gamma_{x_i}))\).

Therefore, Inequality (5) can be rewritten as

\[
(1 - \alpha) \times \frac{d(x_i, x_j)}{d_{\max}} + \alpha \times (p_S(\gamma_{x_i} \cap \gamma_{x_j})) + (1 - \alpha) \times \frac{d(x_j, x_k)}{d_{\max}} + \alpha \times (p_S(\gamma_{x_j} \cap \gamma_{x_k})) \geq (1 - \alpha) \times \frac{d(x_k, x_i)}{d_{\max}} + \alpha \times (p_S(\gamma_{x_k} \cap \gamma_{x_i})).
\]  

(6)

Further simplifying (6), we get

\[
\alpha \times (p(S_{\gamma_S \cup \gamma_{x_k}}) \cap \gamma_{x_j}) + p(S_{\gamma_S \cup \gamma_{x_k}}) \cap \gamma_{x_j} + p(S_{\gamma_S \cup \gamma_{x_k}}) \cap \gamma_{x_j} + p(S_{\gamma_S \cup \gamma_{x_k}}) \cap \gamma_{x_j}) \geq (1 - \alpha) \times (d(x_k, x_i) - (d(x_i, x_j) + d(x_j, x_k))).
\]  

(7)

When \((\gamma_S \cap \gamma_{x_i}) = (\gamma_S \cap \gamma_{x_j}) = (\gamma_S \cap \gamma_{x_k})\), as \(d(x_i, x_j) + d(x_j, x_k) \geq d(x_k, x_i)\), the Right Hand Side (RHS) of Inequality (7) is less than or equal to zero. Now, the Left Hand Side (LHS) of Inequality (7) is always greater than or equal to zero as \(p(S_{\gamma_S \cap \gamma_{x_k}}) \cap \gamma_{x_j} + p(S_{\gamma_S \cap \gamma_{x_k}}) \cap \gamma_{x_j} + p(S_{\gamma_S \cap \gamma_{x_k}}) \cap \gamma_{x_j}) \in [0, 1]\) and \(\alpha \in [0, 1]\). Hence, LHS \(\geq\) RHS, which completes the proof.

**Lemma 3.** If \(|\gamma_S \cap \gamma_{x_i}| \to 0\), \(|\gamma_S \cap \gamma_{x_j}| \to 0\) and \(|\gamma_S \cap \gamma_{x_k}| \to 0\), then Inequality (5) tends to be satisfied.

**Proof.** When \(|\gamma_S \cap \gamma_{x_i}| \to 0\), \(|\gamma_S \cap \gamma_{x_j}| \to 0\) and \(|\gamma_S \cap \gamma_{x_k}| \to 0\), then LHS \to \alpha^-\) and RHS \to 0 for the Inequality (5). As \(\alpha \in [0, 1]\), Inequality (5) tends to be satisfied.
Definition 6. For any dataset \( X \), we define the quantity \( P \) as

\[
P = \min_{x_i, x_j, x_k \in X} \left\{ p_{\gamma x_i \cup \gamma x_k \setminus \gamma x_j} + p_{\gamma x_i \cap \gamma x_k \setminus \gamma x_j} + p_{\gamma x_i \setminus (\gamma x_i \cup \gamma x_k)} + p_{\gamma x_k \setminus (\gamma x_i \cup \gamma x_j)} \right\}.
\]

The following lemma deals with the value of the parameter \( \alpha \in (0, 1] \) for which a relaxed form of the triangle inequality is satisfied for any three data instances in a dataset \( X \), having at least one missing feature among themselves. Now, if there are no missing features among the three data points, then the triangle inequality must hold by Lemma 2. Consequently, if the restrictions on the value of \( \alpha \) presented in the following lemma are satisfied, the presented relaxed form of the inequality will hold for any three data instances in \( X \).

Lemma 4. For any arbitrary constant \( \epsilon \) satisfying \( 0 \leq \epsilon \leq P \), if \( \alpha \geq (1 - \epsilon) \), then the following relaxed form of the triangle inequality

\[
\delta(x_i, x_j) + \delta(x_j, x_k) \geq \delta(x_k, x_i) - \epsilon^2,
\]

is satisfied for any \( x_i, x_j, x_k \in X \).

Proof. As \( \alpha \geq (1 - \epsilon) \), LHS of Inequality (7) \( \geq (1 - \epsilon) \times (p_{\gamma x_i \cup \gamma x_k \setminus \gamma x_j} + p_{\gamma x_i \cap \gamma x_k \setminus \gamma x_j} + p_{\gamma x_i \setminus (\gamma x_i \cup \gamma x_k)} + p_{\gamma x_k \setminus (\gamma x_i \cup \gamma x_j)}) \). Since \( \epsilon \leq P \), we further get that LHS \( \geq (1 - \epsilon)\epsilon \). Moreover, as \( \frac{1}{d_{\text{max}}} (d(x_k, x_i) - (d(x_i, x_j) + d(x_j, x_k))) \leq 1 \), we get RHS of Inequality (7) \( \leq \epsilon \). Therefore, LHS - RHS \( \geq (1 - \epsilon)\epsilon - \epsilon = -\epsilon^2 \). Now, as Inequality (7) is obtained from Inequality (5) after some algebraic manipulation, it must hold that (LHS - RHS) of Inequality (7) = (LHS - RHS) of Inequality (5). Hence, we get

\[
\delta(x_i, x_j) + \delta(x_j, x_k) - \delta(x_k, x_i) \geq -\epsilon^2,
\]

which can be simplified to obtain Inequality (8). This completes the proof.

Let us now elucidate the proposed FWP (and consequently the proposed FWPD measure) by using the following example.

Example 1.

Let \( X \subset \mathbb{R}^3 \) be a dataset consisting of \( n = 5 \) data points, each having three features \( (S = \{1, 2, 3\}) \), some of which (marked by ‘*’) are unobserved. The dataset is presented below (along with the feature observation counts and the observed feature sets for each of the instances).
The pairwise observed distance matrix $A_d$ and the pairwise penalty matrix $A_p$, are as follows:

$$A_d = \begin{bmatrix}
0, & 2, & 3.35, & 1, & 0 \\
2, & 0, & 3.5, & 3.13, & 3.2 \\
3.35, & 3.5, & 0, & 3.04, & 0 \\
1, & 3.13, & 3.04, & 0, & 4.1 \\
0, & 3.2, & 0, & 4.1, & 0
\end{bmatrix} \text{, and } A_p = \begin{bmatrix}
0.3, & 0.6, & 0.3, & 0.3, & 1 \\
0.6, & 0.3, & 0.6, & 0.3, & 0.7 \\
0.3, & 0.3, & 0.3, & 0, & 0.7 \\
1, & 0.7, & 1, & 0.7, & 0.7
\end{bmatrix}.$$  

From $A_d$ it is observed that the maximum pairwise observed distance $d_{max} = 4.1$. Then, the normalized observed distance matrix $A^*_d$ is

$$A^*_d = \begin{bmatrix}
0, & 0.49, & 0.82, & 0.24, & 0 \\
0.49, & 0, & 0.85, & 0.76, & 0.78 \\
0.82, & 0.85, & 0, & 0.74, & 0 \\
0.24, & 0.76, & 0.74, & 0, & 1 \\
0, & 0.78, & 0, & 1, & 0
\end{bmatrix}.$$  

Choosing $\alpha = 0.5$ and using Equation (3) to calculate the FWPD matrix $A_5$, we get:

$$A_5 = 0.5 \times A^*_d + 0.5 \times A_p = \begin{bmatrix}
0.15, & 0.54, & 0.56, & 0.27, & 0.5 \\
0.54, & 0.15, & 0.72, & 0.53, & 0.74 \\
0.56, & 0.72, & 0.15, & 0.52, & 0.5 \\
0.27, & 0.53, & 0.52, & 0, & 0.85 \\
0.5, & 0.74, & 0.5, & 0.85, & 0.35
\end{bmatrix}.$$  

It should be noted that in keeping with the properties of the FWPD described in Subsection 2.1, $A_5$ is a symmetric matrix with the diagonal elements being the smallest entries in their corresponding rows (and columns) and the diagonal element corresponding to the fully observed point $x_4$ being the only zero element.

3. k-means Clustering for Datasets with Missing Features using the proposed FWPD

This section presents a reformulation of the k-means clustering problem for datasets with missing features, using the FWPD measure proposed in Section 2. The k-means problem (a term coined by
MacQueen \[36\]) deals with the partitioning of a set of \( n \) data instances into \( k \) (< \( n \)) clusters so as to minimize the sum of squared within-cluster dissimilarities. The standard heuristic algorithm to solve the k-means problem, referred to as the \textit{k-means algorithm}, was first proposed by Lloyd in 1957 \[37\], and rediscovered by Forgy \[38\]. Starting with \( k \) random assignments of each of the data instances to one of the \( k \) clusters, the k-means algorithm functions by iteratively recalculating the \( k \) cluster centroids and reassigning the data instances to the nearest cluster (the cluster corresponding to the nearest cluster centroid), in an alternating manner. Selim & Ismail \[39\] showed that the k-means algorithm converges to a local optimum of the non-convex optimization problem posed by the k-means problem, when the dissimilarity used is the Euclidean distance between data points.

The proposed formulation of the k-means problem for datasets with missing features using the proposed FWPD measure, referred to as the \textit{k-means-FWPD problem} hereafter, differs from the standard k-means problem not only in that the underlying dissimilarity measure used is FWPD (instead of Euclidean distance), but also in the addition of a new constraint which ensures that a cluster centroid has observable values for exactly those features which are observed for at least one of the points in its corresponding cluster. Therefore, the k-means-FWPD problem to partition the dataset \( X \) into \( k \) clusters (2 \( \leq k < n \)), can be formulated in the following way:

\[
P: \text{minimize } f(U, z_1, \cdots, z_k) = \sum_{i=1}^{n} \sum_{j=1}^{k} u_{i,j} ((1 - \alpha) \times \frac{d(x_i, z_j)}{d_{\text{max}}} + \alpha \times p(x_i, z_j)), \tag{9a}
\]

subject to \( \sum_{j=1}^{k} u_{i,j} = 1 \) \( \forall \; i \in \{1, 2, \cdots, n\} \), \( u_{i,j} \in \{0, 1\} \) \( \forall \; i \in \{1, 2, \cdots, n\}, j \in \{1, 2, \cdots, k\} \), and \( \gamma_{z_j} = \bigcup_{x_i \in C_j} \gamma_{x_i} \). \( \tag{9d} \)

where \( U = [u_{i,j}] \) is the \( n \times k \) real matrix of memberships, \( d_{\text{max}} \) denotes the maximum observed distance between any data point \( x_i \) and any cluster centroid \( z_j (j \in \{1, 2, \cdots, k\}) \), \( \gamma_{z_j} \) denotes the set of observed features for \( z_j \), \( C_j \) denotes the \( j \)-th cluster (corresponding to the centroid \( z_j \)), and it is said that \( x_i \in C_j \) when \( u_{i,j} = 1 \).

\[ \text{3.1. The k-means-FWPD Algorithm} \]

To find a solution to the problem \( P \), which is a non-convex program, we propose a Lloyd’s heuristic-like algorithm based on the FWPD (referred to as \textit{k-means-FWPD algorithm}), as follows:

1. Start with an initial set of cluster assignments \( U \) such that \( \sum_{j=1}^{k} u_{i,j} = 1 \). Set \( t = 1 \).

2. For each of the initial clusters \( C_j^1 \) \( (j = 1, 2, \cdots, k) \), calculate the observed features of the cluster
centroid $z^1_j$ of $C^1_j$ as:

$$z^1_{j,l} = \frac{\sum_{x_i : l \in \gamma_{x_i}} u^1_{i,j} x_{i,l}}{\sum_{x_i : l \in \gamma_{x_i}} u^1_{i,j}} \forall l \in \bigcup_{x_i \in C^1_j} \gamma_{x_i}.$$ 

3. Assign each data point $x_i$ ($i = 1, 2, \cdots, n$) to the cluster corresponding to its nearest (in terms of FWPD) centroid, i.e.

$$u^{t+1}_{i,j} = \begin{cases} 
1, & \text{if } z^t_j = \arg \min_{z \in \{z^1, \cdots, z^k\}} \delta(x_i, z) \\
0, & \text{otherwise}
\end{cases}.$$ 

Set $t = t + 1$.

4. Recalculate the observed features for each of the cluster centroids $z^t_j$ ($j = 1, 2, \cdots, k$) as

$$z^t_{j,l} = \frac{\sum_{x_i : l \in \gamma_{x_i}} u^t_{i,j} x_{i,l}}{\sum_{x_i : l \in \gamma_{x_i}} u^t_{i,j}} \forall l \in \bigcup_{x_i \in C^t_j} \gamma_{x_i}. \quad (10)$$

If $\gamma_{z^t_j} = \gamma_{z^{t-1}_j}$ and $z^t_j = z^{t-1}_j \forall z^t_j$ ($j = 1, 2, \cdots, k$), then stop; otherwise go to Step 3.

3.2. Properties of Problem $P$

In this subsection, we analyse the properties of the problem $P$, which will be used to show that the k-means-FWPD algorithm converges to a local solution of $P$ within a finite number of iterations. Along the lines of [39], we begin by defining an equivalent problem RP to investigate the properties of the problem $P$.

**Definition 7.** The reduced function $F(U)$ of problem $P$ is defined as

$$F(U) = \min_Z \{ f(U, z_1, \cdots, z_k) : Z \text{satisfies constraint } (9d) \},$$

where $Z = \{z_1, \cdots, z_k\}$.

It should be noted that for some values of $U$, $F$ may be unbounded.

**Definition 8.** Let us consider the set $\mathcal{U} = \{ \sum_{j=1}^k u_{i,j} = 1 : u_{i,j} \geq 0 ; i = 1, \cdots, n ; j = 1, \cdots, k \}$. Then the problem RP (a reduction of problem $P$) is given by

$$RP: \min_U F(U), \text{ subject to } U \in \mathcal{U}.$$  

The following lemma and theorem are essential for showing the equivalence of the original problem $P$ and the reduced problem RP.

**Lemma 5.** The reduced objective function $F$ is concave in $U$. 

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Proof. Consider two distinct matrices $U_1$ and $U_2$ and let $\beta \in [0,1]$ be a scalar. Then,

$$F((1-\beta) \times U_1 + \beta \times U_2) = \min_Z \left\{ f((1-\beta)U_1 + \beta U_2, Z_1, \cdots, Z_k) \right\}$$

$$= \min_Z \left\{ (1-\beta) \times f(U_1, Z_1, \cdots, Z_k) + \beta \times f(U_2, Z_1, \cdots, Z_k) \right\} \text{ (by linearity of } U)$$

$$\geq (1-\beta) \times \min_{Z_1} \left\{ f(U_1, Z_1, \cdots, Z_k) \right\} + \beta \times \min_{Z_2} \left\{ f(U_2, Z_1, \cdots, Z_k) \right\}$$

$$= (1-\beta) \times F(U_1) + \beta \times F(U_2).$$

Hence $F$ is concave in $U$.

The following theorem, showing that the extreme points of $U$ satisfy the crisp membership constraint (9c), is borrowed from [39].

**Theorem 6.** The extreme points of $U$ satisfy the constraint (9c).

Proof. Each extreme point of $U$ is associated with a basis. Any basis of the constraints satisfied by $U$ is an identity matrix. Hence, each basic variable will have a value of 1, while the non-basic variables will be zeros. Thus, each of the extreme points of $U$ satisfy constraint (9c).

By Lemma 5 and Theorem 6, it follows that RP is equivalent to P and there exists a solution to RP which is an extreme point of $U$. Therefore, any result pertaining to problem P will transmit to problem RP, and vice-versa.

### 3.3. Partial Optimal Solutions

This subsection deals with the concept of partial optimal solutions of the problem P, to one of which the k-means-FWPD algorithm is shown to converge. The following definition formally presents the concept of a partial optimal solution.

**Definition 9.** A partial optimal solution of problem P, a point $(U^*, Z^*)$, satisfies the following conditions [40]:

$$f(U^*, Z^*) \leq f(U, Z^*) \forall U \in U,$$

and

$$f(U^*, Z^*) \leq f(U^*, Z) \forall Z \text{ satisfying } (9d).$$

To obtain a partial optimal solution of P, the two following subproblems are defined:

- **P1:** Given $\hat{Z}$ satisfying (9d), minimize $f(U, \hat{Z})$ over $U \in U$.

- **P2:** Given $\hat{U} \in U$, minimize $f(\hat{U}, Z)$ over $Z$ satisfying constraint (9d).

The two following lemmas provide conditions for solving the problems P1 and P2, respectively. The subsequent theorem shows that the k-means-FWPD algorithm converges to a partial optimal solution of P.
Lemma 7. Problem P1 is solved if \( u_{i,j} = 1 \) and \( u_{i,j'} = 0 \) \( \forall \ j' \neq j \) when \( \delta(x_i, z_j) \leq \delta(x_i, z_{j'}) \), for all \( j' \neq j \).

Proof. It is clear that the contribution of \( x_i \) to the total objective function is \( \delta(x_i, z_j) \) when \( u_{i,j} = 1 \) and \( u_{i,j'} = 0 \) \( \forall \ j' \neq j \). Since any alternative solution is an extreme point of \( U \), by Theorem 6 it must satisfy \( 9c \). Therefore, the contribution of \( x_i \) to the objective function for an alternative solution will be some \( \delta(x_i, z_{j'}) \geq \delta(x_i, z_j) \). Hence, the contribution of \( x_i \) is minimized by assigning \( u_{i,j} = 1 \) and \( u_{i,j'} = 0 \) \( \forall \ j' \neq j \). This argument holds true for all \( x_i \in X \), i.e. \( \forall \ i \in \{1, \cdots, n\} \). This completes the proof.

Lemma 8. Problem P2 is solved if the observed features of each \( z_j \in Z \) are calculated exactly in the same way as the observed features of \( z_{j'} \) are calculated in Equation (10), i.e. in the following way:

\[
z_{j,l} = \frac{\sum_{x_i: l \in \gamma_{x_i}} u_{i,j} \times x_{i,l}}{\sum_{x_i: l \in \gamma_{x_i}} u_{i,j}} \quad \forall \ l \in \bigcup_{x_i \in C_j} \gamma_{x_i}.
\]

Proof. For fixed \( \hat{U} \in U \), the objective function is minimized when \( \frac{\partial f}{\partial z_{j,l}} = 0 \). Differentiating \( f(\hat{U}, Z) \) w.r.t. \( z_{j,l} \), we get

\[
\frac{\partial f}{\partial z_{j,l}} = \frac{(1 - \alpha)}{d_{max}} \times \sum_{x_i: l \in \gamma_{x_i}} u_{i,j} \left( \frac{2(x_{i,l} - z_{j,l})}{d(x_i, z_j)} \right).
\]

Equating \( \frac{\partial f}{\partial z_{j,l}} = 0 \), and solving for \( z_{j,l} \) gives us

\[
z_{j,l} = \frac{\sum_{x_i: l \in \gamma_{x_i}} u_{i,j} \times x_{i,l}}{\sum_{x_i: l \in \gamma_{x_i}} u_{i,j}}.
\]

Therefore, assigning the observed features for each \( z_j \in Z \) in this way gives an optimal solution of P2.

Theorem 9. The k-means-FWPD algorithm finds a partial optimal solution of P.

Proof. Since Step 3 and Step 4 of the k-means-FWPD algorithm respectively solve P1 and P2, and the algorithm terminates only when the obtained iterate \((U^*, Z^*)\) solves both P1 and P2, it follows that the final solution must be a partial optimal solution of P.

3.4. Convergence of the k-means-FWPD Algorithm

We now show that the k-means-FWPD algorithm converges to the partial optimal solution, within a finite number of iterations. The following theorem is concerned with this.
Theorem 10. The k-means-FWPD algorithm converges to a partial optimal solution of $P$ within a finite number of iterations.

Proof. Let us first note that there are a finite number of extreme points of $U$. Then, an extreme point of $U$ is visited at most once by the algorithm before its termination. Suppose, this is not true, and let $U^{t_1} = U^{t_2}$ for distinct iterations $t_1$ and $t_2$ ($t_1 \neq t_2$) of the algorithm. Applying Step 4 of the algorithm in Subsection 3.1, we get $Z^{t_1+1}$ and $Z^{t_2+1}$ as optimal centroid sets for $U^{t_1}$ and $U^{t_2}$, respectively. Then, $f(U^{t_1}, Z^{t_1+1}) = f(U^{t_2}, Z^{t_2+1})$ since $U^{t_1} = U^{t_2}$. However, the sequence of objective values $f(.,.)$ generated by the algorithm is strictly decreasing; hence, $U^{t_1} \neq U^{t_2}$. Therefore, it is clear from the above argument that the k-means-FWPD algorithm terminates within a finite number of iterations.

3.5. Local Optimality of the Partial Optimal Solutions of $P$

In this subsection, we show that the partial optimal solutions attained by k-means-FWPD algorithm are locally optimal. In the following definition, we present the concept of one-sided directional derivative [4] of the objective function $F$ of RP.

Definition 10. The one-sided directional derivative of $F$ at $U^*$ in the direction $D$ is defined as

$$F'(U^*, D) = \lim_{\theta \to 0^+} (F(U^* + \theta D) - F(U^*))/\theta.$$  

$F'(U^*, D)$ exists for any $D$ at any point $U^*$ and is given by:

$$F'(U^*, D) = \text{trace}(\nabla_U f(U^*, Z)D),$$

with $\nabla_U f(U^*, Z)$ being the vector of partial derivatives $\frac{\partial f(U,Z)}{\partial u_{i,j}}$ evaluated at $U = U^*$.

The following lemma gives the condition for a clustering to be a local optimal solution of RP.

Lemma 11. Let $(U^*, Z^*)$ be a given clustering such that $U^*$ is an extreme point of $U$. Then $U^*$ is a local optimum of problem RP iff

$$F(U^*) = f(U^*, Z^*) \leq \min_U \{f(U, Z^*) : U \in U\}. \quad (11)$$

Proof. Consider the problem RP. If $F(U^*) \leq \min_U \{f(U, Z^*) : U \in U\}$, then, since there exists an unique $Z$ satisfying constraint [9d] for any $U \in U$, for all feasible directions $D$ at $U^*$

$$\text{trace}(\nabla_U f(U^*, Z)D) \geq 0. \quad (12)$$

Hence, $U^*$ is a local optimum of problem RP. Now, to prove the converse, assume $U^*$ is a local optimal solution of RP. Then, for any feasible direction $D$, the inequality in Equation (12) must hold. Hence, since $f(U, Z^*)$ is linear in $U$, $f(U^*, Z^*) \leq \min_U \{f(U, Z^*) : U \in U\}$ must also hold.
The theorem below now shows that a partial optimal solution of problem P is a local optimal solution of RP.

**Theorem 12.** Let \((U^*, Z^*)\) be a partial optimal solution of problem P. Then \(U^*\) is a local optimum of problem RP.

**Proof.** Since \((U^*, Z^*)\) is a partial optimal solution of P, it follows that 
\[
f(U^*, Z^*) \leq f(U, Z^*) \quad \forall \ U \neq U^*,
\]
which is exactly the condition for local optimality of \(U^*\) (Equation (11)). This completes the proof.

Since P and RP have already been shown to be equivalent problems (Section 3.2), the local optimality of \(U^*\) for RP implies the local optimality of \((U^*, Z^*)\) for the problem P. Hence, it is clear that the k-means-FWPD algorithm converges to a local optimal solution of the problem P, within a finite number of iterations.

### 3.6. Time Complexity of the k-means-FWPD Algorithm

In this subsection, we present a brief discussion on the time complexity of the k-means-FWPD algorithm. The k-means-FWPD algorithm consists of four basic steps, which are repeated iteratively. These steps are

i. **Centroid Calculation:** As a maximum of \(m\) features of each centroid must be calculated, the complexity of centroid calculation is at most \(O(kmn)\).

ii. **Distance Calculation:** As each distance calculation involves at most \(m\) features, the observed distance calculation between \(n\) data instances and \(k\) cluster centroids is at most \(O(kmn)\).

iii. **Penalty Calculation:** The penalty calculation between a data point and a cluster centroid involves at most \(m\) summations. Hence, penalty calculation over all possible pairings is at most \(O(kmn)\).

iv. **Cluster Assignment:** The assignment of \(n\) data points to \(k\) clusters consists of the comparisons of the dissimilarities of each point with \(k\) clusters, which is \(O(nk)\).

Therefore, if the algorithm runs for \(t\) iterations, the total computational complexity is \(O(kmnt)\) which is the same as that of the standard k-means algorithm.

### 4. Hierarchical Agglomerative Clustering for Datasets with Missing Features using the proposed FWPD

Hierarchical schemes for data clustering seek to build a multi-level hierarchy of clusters instead of decomposing the entire dataset into disjoint partitions. The two main types of hierarchical clustering...
are *agglomerative* and *divisive hierarchical clustering*. HAC develops a hierarchy of clusters, starting with each data point as a single cluster, by combining two (or more) of the most proximal clusters at one level to obtain a lower number of clusters at the next (higher) level. Divisive hierarchical clustering techniques, on the other hand, starts with the entire dataset as a single cluster, which is then recursively split to obtain higher number of clusters at the next (lower) levels. The solutions obtained by hierarchical clustering algorithms are often represented in the form of trees known as *dendograms*, where the height of each node is inversely proportional to the proximity between its offspring. A partitioning of the data into $k$ clusters can be obtained from the dendogram as the partitioning at the level which has exactly $k$ nodes. However, these methods cannot be directly applied to datasets with missing features. Therefore, in this section, we develop variants of HAC methods, based on the proposed FWPD measure.

Various proximity measures may be used to merge the clusters in an agglomerative clustering method. Modifications of the three most popular of such proximity measures (SL, CL and AL) so as to have FWPD as the underlying dissimilarity measure, are as follows:

i. *Single Linkage with FWPD (SL-FWPD)*: The SL between two clusters $C_i$ and $C_j$ is $\min\{\delta(x_i, x_j) : x_i \in C_i, x_j \in C_j\}$.

ii. *Complete Linkage with FWPD (CL-FWPD)*: The CL between two clusters $C_i$ and $C_j$ is $\max\{\delta(x_i, x_j) : x_i \in C_i, x_j \in C_j\}$.

iii. *Average Linkage with FWPD (AL-FWPD)*: $\frac{1}{|C_i| \times |C_j|} \sum_{x_i \in C_i} \sum_{x_j \in C_j} \delta(x_i, x_j)$ is the AL between two clusters $C_i$ and $C_j$, where $|C_i|$ and $|C_j|$ are respectively the number of instances in the clusters $C_i$ and $C_j$.

4.1. The HAC-FWPD Algorithm

To achieve hierarchical clusterings in the presence of unstructured missingness, the HAC method based on SL-FWPD, CL-FWPD, or AL-FWPD, referred to as the *HAC-FWPD algorithm* hereafter, is as follows:

1. Set $X_0 = X$. Compute all pairwise dissimilarities $\delta(x_i, x_j)$, $x_i, x_j \in X_0$ between all elements of $X_0$ to construct the dissimilarity matrix $D_0$. Set $t = 0$.

2. Search $D_t$ for all the pairs of points $\{(x_{i1}, x_{j1}), (x_{i2}, x_{j2}), \ldots, (x_{ik}, x_{jk})\}$ having dissimilarity $\delta_t$ (the smallest non-zero element in $D_t$) with each other, i.e. $\delta(x_{ir}, x_{jr}) = \delta_t \ \forall \ r \in \{1, 2, \ldots, k\}$.

3. Merge any pair of elements in this list, $(x_{ir}, x_{jr})$ say, into a single group $G = \{x_{ir}, x_{jr}\}$. Define $X_{t+1} = (X_t \setminus \{x_{ir}, x_{jr}\}) \cup G$. Define $D_{t+1}$ on $X_{t+1} \times X_{t+1}$ as $D_{t+1}(A, B) = D_t(A, B) \ \forall \ A, B \neq G$.
and $D_{t+1}(A,G) = D_t(G,A) = L(G,A)$, where

$$L(G,A) = \begin{cases} 
\min_{x_i \in G, x_j \in A} \delta(x_i, x_j) & \text{for SL-FWPD}, \\
\max_{x_i \in G, x_j \in A} \delta(x_i, x_j) & \text{for CL-FWPD}, \\
\frac{1}{|G| \cdot |A|} \sum_{x_i \in G} \sum_{x_j \in A} \delta(x_i, x_j) & \text{for AL-FWPD}.
\end{cases}$$

Set $t = t + 1$.

4. Repeat Steps 2-3 until $X_t$ contains a single element.

FWPD being the underlying dissimilarity measure (instead of other metrics such as the Euclidean distance), the HAC-FWPD algorithm can be directly applied to obtain SL, CL, or AL based hierarchical clustering of datasets with missing feature values.

4.2. Time Complexity of the HAC-FWPD Algorithm

Irrespective of whether SL-FWPD, AL-SWPD or CL-FWPD is used as the proximity measure, the HAC-FWPD algorithm consists of three following basic steps:

i. **Distance Calculation**: As each distance calculation involves at most $m$ features, the calculation of all pairwise observed distances among $n$ data instances is at most $O(n^2 m)$.

ii. **Penalty Calculation**: The penalty calculation between a data point and a cluster centroid involves at most $m$ summations. Hence, penalty calculation over all possible pairings is at most $O(n^2 m)$.

iii. **Cluster Merging**: The merging of two clusters takes place in each of the $n-1$ steps of the algorithm, and each merge at most has a time complexity of $O(n^2)$.

Therefore, assuming $m \ll n$, the total computational complexity of the HAC-FWPD algorithm is $O(n^3)$ which is the same as that of the standard HAC algorithm based on SL, CL or AL.

5. Experimental Results

In this section, we report the results of several experiments carried out to validate the merit of the proposed k-means-FWPD and HAC-FWPD clustering algorithms. In the following subsection, we describe the philosophy of the experiments carried out to validate the proposed techniques. The subsequent subsections present the results of the experiments for the k-means-FWPD algorithm and the HAC-FWPD algorithm, respectively.
5.1. Experiment Philosophy

Normalized Mutual Information (NMI) and Adjusted Rand Index (ARI) are two popular validity indices used to judge the merit of clustering algorithms. When the true class labels are known, NMI and ARI provide measures of the similarity between the cluster partition obtained by a clustering technique and the true class labels. Therefore, high values of NMI or ARI are thought to indicate better clusterings. But, the class labels may not always be in keeping with the natural cluster structure of the dataset. In such cases, good clusterings are likely to achieve lower values of these indices compared to possibly erroneous partitions (which are more akin to the class labels). However, the purpose of our experiments is to find out how close the clusterings obtained by the proposed methods (and the contending techniques) are to the clusterings obtained by the standard algorithms (k-means algorithm and HAC algorithm); the proposed methods (and its contenders) being run on the datasets with missingness, while the standard methods are run on corresponding fully observed datasets. Hence, the clusterings obtained by the standard algorithms are used as the ground-truths using which the NMI and ARI values are calculated for the proposed methods (and their contenders). Two indices are used instead of a single one to compensate for certain biases that the individual indices may have. The performances of ZI, MI, kNNI (with \( k \in \{3, 5, 10, 20\} \)) and SVDI (using the most significant 10% of the Eigenvectors) have been used for comparison with the proposed methods. The variant of MI that we use for these experiments differs from the traditional technique in that we use the average of the averages for individual classes, instead of the overall average. This is done to minimize the effects of severe class imbalances that may exist in the datasets.

Since labelled data may not be available for most practical clustering applications, we do not attempt to find the optimal value of the parameter \( \alpha \) using labelled data instances. Instead, we conduct two sets of experiments for \( \alpha = 0.25 \) and \( \alpha = 0.5 \), to study the dependence on the choice of \( \alpha \). The first choice is based on the fact that about 25% of the features are removed from each dataset, while the second choice aims to give equal weightage to both the terms of FWPD (see Equation 3). The results for both sets of experiments are comparable. and we report the results for the former choice of \( \alpha \) in the following subsections. While the performance seems to have low dependence on the choice of the \( \alpha \) parameter, a lower value of \( \alpha \) may be more useful when small fraction of features are missing and a higher value may be used when a very larger fraction of features are unobserved.

It should also be noted that in all the reported experiments, we have used the same sets of missing patterns (and the same sets of initial seeds as well for partitional clustering) for all the contending methods on a particular dataset. In fact, this same set of initial seeds (for the dataset in question) was also used for the runs of the standard k-means algorithm on the fully observed dataset (corresponding to the dataset in question). The patterns of missingness (and initial seeds) are kept the same for all algorithms for a particular dataset so that any difference in the performance of these methods may be
attributed to their internal learning mechanisms only.

5.2. Experiments with the k-means-FWPD Algorithm

5.2.1. UCI Datasets with Random Feature Removal

We take 12 datasets from the well-known University of California at Irvine (UCI) repository and randomly remove up to \( \frac{m}{2} \) (\( m \) being the dimension of the fully observed data instances) features from each of the data points. Thus, an average of about \( \frac{m}{4} \) of the features are missing from each instance. Each of the features of each dataset are normalized so as to have zero mean and unit standard deviation. The details of these 12 datasets are listed in Table 1.

Table 1: Details of the 12 UCI datasets

| Dataset       | #Instances | #Features | #Classes |
|---------------|------------|-----------|----------|
| Balance       | 625        | 4         | 3        |
| Cardio        | 2126       | 21        | 3        |
| Chronic Kidney| 800        | 24        | 2        |
| Glass         | 214        | 9         | 6        |
| Iris          | 150        | 4         | 3        |
| Libras        | 360        | 90        | 15       |
| Monk1         | 556        | 6         | 2        |
| Monk2         | 601        | 6         | 2        |
| Monk3         | 554        | 6         | 2        |
| Pendigits     | 10992      | 16        | 10       |
| Seeds         | 210        | 7         | 3        |
| Vehicle       | 94         | 18        | 4        |

Alongside the proposed k-means-FWPD algorithm, we run the standard k-means algorithm on the datasets obtained after ZI, MI, SVDI and kNNI for 50 different runs, using the same set of initial cluster assignments and the same patterns of missingness for each method in any particular run. The number of clusters is assumed to be same as the number of classes. The results of the experiments are listed in terms of average NMI and ARI values, in Table 2. Only the best results for kNNI are reported, along with the best \( k \) values.

It is seen from Table 2 that the k-means-FWPD algorithm is able to achieve the best results, in terms of both NMI and ARI values, on 8 out of the 12 tested datasets. kNNI, on the other hand, is able to achieve the best performance on 4 out of the 12 tested datasets whereas ZI and MI (which exhibit similar performance) never achieve the best results. The failure of the proposed method to achieve the
Table 2: Results of the k-means-FWPD algorithm on UCI datasets

| Dataset        | Index | k-means-FWPD | ZI    | MI    | SVDI  | kNNI  | Best k (for kNNI) |
|----------------|-------|--------------|-------|-------|-------|-------|------------------|
| Balance        | NMI   | **0.2656**   | 0.2619| 0.2620| 0.1589| 0.2432| 20               |
|                | ARI   | **0.3199**   | 0.3133| 0.3137| 0.1729| 0.2937|                  |
| Cardio         | NMI   | 0.5231       | 0.4691| 0.4690| 0.4299| **0.6025**      | 10               |
|                | ARI   | 0.6102       | 0.5514| 0.5509| 0.5061| **0.6436**      |                  |
| Chronic Kidney | NMI   | **0.3137**   | 0.3121| 0.3123| 0.2871| 0.3113| 3                |
|                | ARI   | **0.3987**   | 0.3936| 0.3939| 0.3677| 0.3877|                  |
| Glass          | NMI   | 0.4317       | 0.4270| 0.4270| 0.3691| **0.5287**      | 5                |
|                | ARI   | 0.4261       | 0.4206| 0.4206| 0.3604| **0.5364**      |                  |
| Iris           | NMI   | **0.5269**   | 0.4943| 0.4940| 0.5016| 0.5164| 10               |
|                | ARI   | **0.6855**   | 0.5273| 0.5271| 0.5336| 0.6423|                  |
| Libras         | NMI   | **0.6815**   | 0.6757| 0.6757| 0.6379| 0.6653| 10               |
|                | ARI   | **0.6047**   | 0.5969| 0.5966| 0.5410| 0.5963|                  |
| Monk1          | NMI   | **0.2107**   | 0.2102| 0.2101| 0.1671| 0.2008| 20               |
|                | ARI   | **0.2714**   | 0.2704| 0.2701| 0.2198| 0.2595|                  |
| Monk2          | NMI   | **0.2558**   | 0.2510| 0.2509| 0.1686| 0.2398| 20               |
|                | ARI   | **0.3261**   | 0.3228| 0.3225| 0.2199| 0.3091|                  |
| Monk3          | NMI   | **0.2559**   | 0.2548| 0.2548| 0.1745| 0.2404| 20               |
|                | ARI   | **0.3291**   | 0.3275| 0.3276| 0.2280| 0.3099|                  |
| Pendigits      | NMI   | 0.4305       | 0.2193| 0.2193| 0.3711| **0.4244**      | 3                |
|                | ARI   | 0.4076       | 0.1644| 0.1644| 0.3161| **0.2457**      |                  |
| Seeds          | NMI   | 0.5134       | 0.4872| 0.4875| 0.5625| **0.7086**      | 10               |
|                | ARI   | 0.5992       | 0.5739| 0.5743| 0.6448| **0.7944**      |                  |
| Vehicle        | NMI   | **0.6150**   | 0.5968| 0.5972| 0.6027| 0.5942| 10               |
|                | ARI   | **0.6405**   | 0.6186| 0.6199| 0.6265| 0.6047|                  |

best performance on 4 of the 12 datasets is possibly due to these datasets possessing special structural aspects which make them more suitable for kNNI. More conclusive statements about this can only be made after further experimentation.

5.2.2. MNIST Datasets with Random Missing Patches

We also conduct experiments on 3 two-class and a three-class dataset constructed by randomly picking 100 images from the Special Dataset 1 and 500 images from the Special Dataset 3 of the MNIST dataset [45] for each class. These datasets are constructed so that the contending classes represent digits with structural similarities. The details of the datasets are listed in Table 3.

A 14 × 14 square patch of pixels is removed at random from each of the images in the datasets. The images of some of the digits, after the removal of the square patch are shown in Figure 2.
Table 3: Details of the 4 MNIST datasets

| Dataset          | Classes | #Instances |
|------------------|---------|------------|
| MNIST1vs7        | 1, 7    | 1200       |
| MNIST3vs8        | 3, 8    | 1200       |
| MNIST4vs9        | 4, 9    | 1200       |
| MNIST0vs6vs9     | 0, 6, 9 | 1800       |

Figure 2: Some of the digits from the MNIST dataset, after the removal of random $14 \times 14$ square patches

The k-means-FWPD algorithm is run 50 times on each of the datasets, alongside 50 runs each of the standard k-means algorithm on the datasets obtained after applying ZI, MI, SVDI and kNNI to each of the datasets. Identical sets of initial cluster assignments and patterns of missingness are used for each of the techniques. The results of the experiments are listed in terms of average NMI and ARI values, in Table 4. Only the best results for kNNI are reported, along with the best $k$ values.

An inspection of Table 4 shows that the k-means-FWPD algorithm outperforms the contending methods on 2 out of the 3 two-class datasets, namely MNIST1vs7 and MNIST3vs8. Though ZI and MI achieve the best performance in terms of ARI for the MNIST3vs8 dataset, the performance of the k-means-FWPD algorithm on this dataset is the best in terms of NMI. Such a close contention is also seen between the proposed method, ZI and MI on the three-class MNIST0vs6vs9 dataset; but the k-means-FWPD algorithm emerged victorious by a small margin. It is interesting to note that the performances achieved by ZI and MI are identical for all the 4 datasets. This is probably because most of the pixels in each of the images are zero-valued.
Table 4: Results of the k-means-FWPD algorithm on the MNIST datasets

| Dataset | Index | k-means-FWPD | ZI  | MI  | SVDI | kNNI | Best k (for kNNI) |
|---------|-------|--------------|-----|-----|------|------|-------------------|
| MNIST1vs7 | NMI  | 0.5887       | 0.5870 | 0.5870 | 0.5822 | 0.5226 | 3                 |
|         | ARI  | 0.6955       | 0.6837 | 0.6837 | 0.6889 | 0.6284 |                   |
| MNIST3vs8 | NMI  | 0.5296       | 0.5291 | 0.5291 | 0.5204 | 0.4814 | 5                 |
|         | ARI  | 0.6330       | 0.6327 | 0.6327 | 0.6237 | 0.5836 |                   |
| MNIST4vs9 | NMI  | 0.5653       | 0.5651 | 0.5651 | 0.5500 | 0.5307 | 5                 |
|         | ARI  | 0.6691       | 0.6692 | 0.6692 | 0.6556 | 0.6358 |                   |
| MNIST0vs6vs9 | NMI | 0.5948       | 0.5943 | 0.5943 | 0.5901 | 0.5237 | 20                |
|         | ARI  | 0.6820       | 0.6814 | 0.6814 | 0.6763 | 0.6106 |                   |

5.3. Experiments with the HAC-FWPD Algorithm

5.3.1. UCI Datasets with Random Feature Removal

We take the 12 UCI datasets listed in Table 1 and as before, randomly remove up to \( \frac{m}{4} \) features from each of the data instances so that an average of about \( \frac{m}{4} \) of the features are missing from each instance. Each of the features of each dataset are normalized so as to have zero mean and unit standard deviation. We then run the HAC-FWPD algorithm (with AL-FWPD as the proximity measure), alongside the standard HAC algorithm (with AL as the proximity measure) on the datasets obtained after applying ZI, MI, SVDI and kNNI, each for 20 independent runs with the same patterns of missingness for each of the techniques. AL is preferred here over SL and CL as it is observed to generally achieve clustering having higher NMI and ARI values. The results of the experiments are listed in terms of average NMI and ARI values, in Table 5. We only report the best results for kNNI, along with the best \( k \) values.

It is seen from Table 5 that the HAC-FWPD algorithm is able to achieve the best results in terms of NMI on 9 out of the 12 tested datasets. It also achieves the best results on 11 out of the 12 datasets, in terms of ARI. kNNI is able to achieve the best results on one of the 12 datasets, while ZI and SVDI achieve the highest NMI values on one dataset each.

5.3.2. Reuters RCV1 Dataset with Random Feature Removal

As it is well known that document clustering lends itself well to HAC, we randomly pick 50 documents (encoded in the bag-of-words format) from each of the 6 classes of the Reuters RCV1 document dataset and randomly remove up to \( \frac{m}{4} \) words (or numerals) from each of the documents so that an average of about \( \frac{m}{4} \) words are missing from each document. Each feature (representing words or
| Dataset         | Index | HAC-FWPD | ZI   | MI   | SVDI | kNNI | Best k (for kNNI) |
|-----------------|-------|----------|------|------|------|------|-------------------|
| Balance         | NMI   | 0.1154   | 0.1117 | 0.1117 | 0.1028 | 0.0713 | 5                 |
|                 | ARI   | 0.1030   | 0.0514 | 0.0515 | 0.0861 | 0.0720 |                  |
| Cardio          | NMI   | 0.5097   | 0.4501 | 0.4503 | 0.4275 | 0.0231 | 10                |
|                 | ARI   | 0.5644   | 0.4910 | 0.4913 | 0.4624 | 0.0234 |                  |
| Chronic Kidney  | NMI   | 1.0000   | 0.9581 | 0.9581 | 0.9163 | 0.0033 | 3                 |
|                 | ARI   | 1.0000   | 0.9665 | 0.9665 | 0.9331 | 0.0019 |                  |
| Glass           | NMI   | 0.6577   | 0.6600 | 0.6589 | 0.6388 | 0.0937 | 3                 |
|                 | ARI   | 0.7136   | 0.6925 | 0.6923 | 0.6731 | 0.0171 |                  |
| Iris            | NMI   | 0.8791   | 0.8676 | 0.8677 | 0.8903 | 0.7074 | 10                |
|                 | ARI   | 0.9283   | 0.9185 | 0.9189 | 0.9263 | 0.5583 |                  |
| Libras          | NMI   | 0.9293   | 0.0963 | 0.0963 | 0.7017 | 0.5078 | 3                 |
|                 | ARI   | 0.8743   | 0.0002 | 0.0002 | 0.4316 | 0.2068 |                  |
| Monk1           | NMI   | 0.1643   | 0.0068 | 0.0068 | 0.1138 | 0.0071 | 10                |
|                 | ARI   | 0.2028   | 0.0011 | 0.0011 | 0.1408 | 0.0022 |                  |
| Monk2           | NMI   | 0.1169   | 0.0543 | 0.0542 | 0.1027 | 0.0044 | 20                |
|                 | ARI   | 0.1340   | 0.0566 | 0.0567 | 0.1230 | 0.0115 |                  |
| Monk3           | NMI   | 0.2202   | 0.0528 | 0.0528 | 0.1562 | 0.0192 | 20                |
|                 | ARI   | 0.2741   | 0.0535 | 0.0535 | 0.1948 | 0.0140 |                  |
| Pendigits       | NMI   | 0.7977   | 0.4275 | 0.4276 | 0.4240 | 0.5971 | 5                 |
|                 | ARI   | 0.7965   | 0.2246 | 0.2246 | 0.2235 | 0.3735 |                  |
| Seeds           | NMI   | 0.6398   | 0.4917 | 0.4923 | 0.5508 | 0.6428 | 3                 |
|                 | ARI   | 0.6255   | 0.3978 | 0.3991 | 0.4975 | 0.6357 |                  |
| Vehicle         | NMI   | 0.7324   | 0.4078 | 0.4081 | 0.6734 | 0.1609 | 3                 |
|                 | ARI   | 0.7786   | 0.2407 | 0.2400 | 0.7051 | 0.0887 |                  |

The dataset thus obtained is clustered using the HAC-FWPD algorithm with SL-FWPD, AL-FWPD, and CL-FWPD as the underlying proximity measures. Alongside the HAC-FWPD algorithms, we also run the standard HAC algorithm (SL, AL as well as CL based variants) on the fully observed documents and on the datasets obtained by filling in the missing words using ZI, MI, SVDI and kNNI. Each technique is run for 20 independent runs with the same patterns of randomly missing words. The results obtained are summarized in Table 6 in terms of both average NMI and ARI values. It is seen that the HAC-FWPD algorithm achieves the highest NMI and ARI values with SL-FWPD, AL-FWPD as well as CL-FWPD as the underlying proximity measures, suggesting that FWPD is better able to handle the missingness compared to ZI, MI, SVDI and kNNI.
Table 6: Results of the HAC-FWPD algorithm on the Reuters RCV1 datasets

| Proximity Measure | Index | HAC-FWPD | ZI   | MI   | SVDI | kNNI   | Best k (for kNNI) |
|-------------------|-------|----------|------|------|------|--------|------------------|
| SL/SL-FWPD        | NMI   | 0.8021   | 0.8003| 0.8003| 0.6050| 0.1373 | All*             |
|                   | ARI   | 0.7952   | 0.7742| 0.7742| 0.5525| 0.0008 |                  |
| AL/AL-FWPD        | NMI   | 0.8021   | 0.8003| 0.8003| 0.6050| 0.1409 | All*             |
|                   | ARI   | 0.7952   | 0.7742| 0.7742| 0.5525| 0.0023 |                  |
| CL/CL-FWPD        | NMI   | 0.8021   | 0.8003| 0.8003| 0.6050| 0.1409 | All*             |
|                   | ARI   | 0.7952   | 0.7742| 0.7742| 0.5525| 0.0023 |                  |

* kNNI achieves the same results for all values of $k \in \{3, 5, 10, 20\}$.

6. Conclusions

In this paper, we have proposed the FWPD measure as an interesting alternative to imputation and marginalization approaches to handle the problem of missing features in data analysis. Based on the FWPD, we have put forth the k-means-FWPD and the HAC-FWPD algorithms, which are directly applicable to datasets with missing features. We have conducted extensive experimentation on the new techniques using various benchmark datasets and found the new approach to produce generally better results (for both partitional as well as hierarchical clustering) compared to some of the popular imputation methods which are generally used to handle the missing feature problem. We have also presented an appendix dealing with an extension of the FWPD measure to problems with absent features and show that this modified form of FWPD is a semimetric.

The experimental results indicate that (as far as data clustering is concerned) the performance of the proposed FWPD is almost always better than those of the ZI, MI and SVDI techniques. kNNI, on the other hand, proves to be a good contender for partitional clustering, but not in the case of hierarchical clustering. In contrast, the proposed FWPD measure was able to achieve competitive results on all the tested datasets, for both partitional as well as hierarchical clustering algorithms. However, it must be stressed, that the performance of all these methods, including the FWPD based ones, can vary depending on the structure of the dataset concerned, the choice of the proximity measure used (for HAC), and the pattern and extent of missingness plaguing the data. Fortunately, the $\alpha$ parameter embedded in FWPD can be varied in accordance with the extent of missingness to achieve desired results. Even though the performance of the proposed PDM seems to have low dependence on the
choice of $\alpha$, it may be useful to choose a high value of $\alpha$ when a large fraction of the features are unobserved, and to choose a smaller value when only a few of the features are missing. However, in the presence of a sizable amount of missingness and the absence of ground-truths to validate the merit of the achieved clusterings, it is safest to choose a medium value of $\alpha$, such as $\alpha = 0.5$.

An obvious follow-up to this work is the application of the proposed PDM variant to practical clustering problems which are characterized by large fractions of unobserved data that arise in various fields such as economics, psychiatry, web-mining, etc. Studies can be undertaken to better understand the effects that the choice of $\alpha$ has on the clustering results. Another rewarding topic of research is the investigation of the abilities of the FWPD variant for absent features (see Appendix A) by conducting proper experiments using benchmark applications characterized by this rare form of missingness (structural missingness).

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References

[1] L. S. Chan, O. J. Dunn, Journal of the American Statistical Association 67 (1972) 473–477.
[2] D. B. Rubin, Biometrika 63 (1976) 581–592.
[3] G. Chechik, G. Heitz, G. Elidan, P. Abbeel, D. Koller, Journal of Machine Learning Research 9 (2008) 1–21.
[4] E. Acuña, C. Rodriguez, in: D. Banks, F. R. McMorris, P. Arabie, W. Gaul (Eds.), Classification, Clustering, and Data Mining Applications, Studies in Classification, Data Analysis, and Knowledge Organisation, Springer Berlin Heidelberg, 2004, pp. 639–647.
[5] R. J. A. Little, D. B. Rubin, Statistical Analysis with Missing Data, John Wiley & Sons, Inc., New York, 1987.
[6] J. L. Schafer, J. W. Graham, Psychological Methods 7 (2002) 147–177.
[7] W. Zhang, Y. Yang, Q. Wang, International Journal of Software Engineering and Knowledge Engineering 22 (2012) 185–202.
[8] J. L. Schafer, Analysis of Incomplete Multivariate Data, CRC Press, 1997.
[9] A. R. T. Donders, G. J. M. G. van der Heijden, T. Stijnen, K. G. M. Moons, Journal of Clinical Epidemiology 59 (2006) 1087–1091.

[10] J. K. Dixon, Systems, Man and Cybernetics, IEEE Transactions on 9 (1979) 617–621.

[11] J. W. Grzymala-Busse, M. Hu, in: Rough Sets and Current Trends in Computing, Springer, pp. 378–385.

[12] D. B. Rubin, Multiple Imputation for Nonresponse in Surveys, John Wiley & Sons, 1987.

[13] W. R. Gilks, S. Richardson, D. J. Spiegelhalter, Markov chain Monte Carlo in practice 1 (1996) 1–19.

[14] F. Chen, in: Proceedings of the SAS Global Forum 2013 Conference, SAS Institute Inc., 2013, pp. 1–23.

[15] N. J. Horton, S. R. Lipsitz, The American Statistician 55 (2001) 244–254.

[16] C. Barceló, in: Working Paper Series, Banco de España, 2008.

[17] I. Myrtveit, E. Stensrud, U. H. Olsson, Software Engineering, IEEE Transactions on 27 (2001) 999–1013.

[18] A. P. Dempster, D. B. Rubin, Part I: Introduction, volume 2, New York: Academic Press, 1983, pp. 3–10.

[19] S. Ahmad, V. Tresp, in: S. Hanson, J. Cowan, C. Giles (Eds.), Advances in Neural Information Processing Systems 5, Morgan-Kaufmann, 1993, pp. 393–400.

[20] Q. Wang, J. N. K. Rao, Scandinavian Journal of Statistics 29 (2002) 563–576.

[21] Q. Wang, J. N. K. Rao, The Annals of Statistics 30 (2002) 896–924.

[22] O. Troyanskaya, M. Cantor, G. Sherlock, P. Brown, T. Hastie, R. Tibshirani, D. Botstein, R. B. Altman, Bioinformatics 17 (2001) 520–525.

[23] T. H. Bo, B. Dysvik, I. Jonassen, Nucleic Acid Research 32 (2004).

[24] M. S. B. Sehgal, I. Gondal, L. S. Dooley, Bioinformatics 21 (2005) 2417–2423.

[25] M. S. B. Sehgal, I. Gondal, L. S. Dooley, in: Hybrid Intelligent Systems, 2004. HIS’04. Fourth International Conference on, IEEE, 2004, pp. 274–279.

[26] M. Ouyang, W. J. Welsh, P. Georgopoulos, Bioinformatics 20 (2004) 917–923.
[27] D. F. Heitjan, S. Basu, The American Statistician 50 (1996) 207–213.

[28] B. M. Marlin, Missing Data Problems in Machine Learning, Ph.D. thesis, University of Toronto, 2008.

[29] S. Krause, R. Polikar, in: Proceedings of the International Joint Conference on Neural Networks, 2003, volume 1, IEEE, pp. 553–558.

[30] P. Juszczak, R. P. W. Duin, in: Multiple Classifier Systems, Springer, 2004, pp. 92–101.

[31] L. Nanni, A. Lumini, S. Brahnam, Artificial Intelligence in Medicine 55 (2012) 37–50.

[32] R. J. Hathaway, J. C. Bezdek, Systems, Man, and Cybernetics: Part B: Cybernetics, IEEE Transactions on 31 (2001) 735–744.

[33] K. L. Wagstaff, in: Proceedings of the Meeting of the International Federation of Classification Societies, pp. 649–658.

[34] K. L. Wagstaff, V. G. Laidler, in: Astronomical Data Analysis Software and Systems XIV, ASP Conference Series, Astronomical Society of the Pacific, 2005, pp. 172–176.

[35] L. Himmelspach, S. Conrad, in: Digital Information Management (ICDIM), 2010 Fifth International Conference on, pp. 19–28.

[36] J. MacQueen, in: Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability, volume 1, University of California Press, pp. 281–297.

[37] S. P. Lloyd, Information Theory, IEEE Transactions on 28 (1982) 129–137.

[38] E. W. Forgy, Biometrics 21 (1965) 768–769.

[39] S. Z. Selim, M. A. Ismail, Pattern Analysis and Machine Intelligence, IEEE Transactions on 6 (1984) 81–87.

[40] R. E. Wendel, A. P. Hurter Jr., Operations Research 24 (1976) 643–657.

[41] L. S. Lasdon, Optimization theory for Large Systems, Courier Corporation, 2013.

[42] N. X. Vinh, J. Epps, J. Bailey, Journal of Machine Learning Research 11 (2010) 2837–2854.

[43] L. Hubert, P. Arabie, Journal of Classification 2 (1985) 193–218.

[44] M. Lichman, UCI machine learning repository, 2013. URL: http://archive.ics.uci.edu/ml
APPENDIX

Appendix A. Extending the FWPD to problems with Absent Features

This appendix discusses an extension of the proposed FWPD to the case of absent features or structural missingness. As discussed earlier in Section 1.4, the fundamental difference between the problems of missing and absent features is that two points observed in the same subspace and having identical observed features should (unlike the missing data problem) essentially be considered identical instances in the case of absent features, as the unobserved features are known to be non-existent. But, in case of the unobserved features being merely unknown (rather than being non-existent), such data points should be considered distinct because the unobserved features are likely to have distinct values (making the points distinct when completely observed). Keeping this in mind, we can modify the proposed FWPD (essentially modifying the proposed FWP) as defined in the following text to serve as a dissimilarity measure for structural missingness.

Let the dataset $X_{\text{abs}}$ consist of $n$ data instances $x_i$ ($i \in \{1, 2, \cdots, n\}$). Let $\zeta_{x_i}$ denote the set of features on which the data point $x_i \in X_{\text{abs}}$ is defined.

**Definition 11.** The FWP between the instances $x_i$ and $x_j$ in $X_{\text{abs}}$ is defined as

$$p_{\text{abs}}(x_i, x_j) = \frac{\sum_{l \in (\zeta_{x_i} \cup \zeta_{x_j}) \setminus (\zeta_{x_i} \cap \zeta_{x_j})} \nu_l}{\sum_{l' \in \zeta_{x_i} \cup \zeta_{x_j}} \nu_{l'}}$$

(A.1)

where $\nu_s \in (0, n]$ is the number of instances in $X_{\text{abs}}$ that are characterised by the feature $s$. Like in the case of unstructured missingness, this FWP also extracts greater penalty for the non-existence of commonly features.

Then, the definition of the FWPD modified for structural missingness is as follows.

**Definition 12.** The FWPD between $x_i$ and $x_j$ in $X_{\text{abs}}$ is

$$\delta_{\text{abs}}(x_i, x_j) = (1 - \alpha) \times \frac{d(x_i, x_j)}{d_{\text{max}}} + \alpha \times p_{\text{abs}}(x_i, x_j),$$

(A.2)

where $\alpha \in (0, 1)$ is a parameter which determines the relative importance between the two terms and $d(x_i, x_j)$ and $d_{\text{max}}$ retain their former definitions (but, in the context of structural missingness).
Now, having modified the FWPD to handle structural missingness, we show in the following theorem that the modified FWPD is a semimetric.

**Theorem 13.** The FWPD for absent features is a semimetric, i.e. it satisfies the following important properties:

i. $\delta_{\text{abs}}(x_i, x_j) \geq 0 \forall x_i, x_j \in X_{\text{abs}}$,

ii. $\delta_{\text{abs}}(x_i, x_j) = 0$ iff $x_i = x_j$, i.e. $\zeta_{x_i} = \zeta_{x_j}$ and $x_{i,l} = x_{j,l} \forall l \in \zeta_{x_i}$,

iii. $\delta_{\text{abs}}(x_i, x_j) = \delta_{\text{abs}}(x_j, x_i) \forall x_i, x_j \in X_{\text{abs}}$.

**Proof.**

i. From Equation (A.1) we can see that $p_{\text{abs}}(x_i, x_j) \geq 0 \forall x_i, x_j \in X_{\text{abs}}$ and Equation (1) implies that $d(x_i, x_j) \geq 0 \forall x_i, x_j \in X_{\text{abs}}$. Hence, it follows that $\delta_{\text{abs}}(x_i, x_j) \geq 0 \forall x_i, x_j \in X_{\text{abs}}$.

ii. It is easy to see from Equation (A.1) that $p_{\text{abs}}(x_i, x_i) = 0$ iff $\zeta_{x_i} = \zeta_{x_j}$. Now, if $x_{i,l} = x_{j,l} \forall l \in \zeta_{x_i}$, then $d(x_i, x_j) = 0$. Hence, $\delta_{\text{abs}}(x_i, x_j) = 0$ when $\zeta_{x_i} = \zeta_{x_j}$ and $x_{i,l} = x_{j,l} \forall l \in \zeta_{x_i}$. The converse is also true as $\delta_{\text{abs}}(x_i, x_j) = 0$ implies $\zeta_{x_i} = \zeta_{x_j}$ and $d(x_i, x_j) = 0$; the latter in turn implying that $x_{i,l} = x_{j,l} \forall l \in \zeta_{x_i}$.

iii. From Equation (A.2) we have

$$\delta_{\text{abs}}(x_i, x_j) = (1 - \alpha) \times \frac{d(x_i, x_j)}{d_{\text{max}}} + \alpha \times p_{\text{abs}}(x_i, x_j),$$

and

$$\delta_{\text{abs}}(x_j, x_i) = (1 - \alpha) \times \frac{d(x_j, x_i)}{d_{\text{max}}} + \alpha \times p_{\text{abs}}(x_j, x_i).$$

But, $d(x_i, x_j) = d(x_j, x_i)$ and $p_{\text{abs}}(x_i, x_j) = p(x_j, x_i) \forall x_i, x_j \in X_{\text{abs}}$ (by definition). Therefore, it can be easily seen that $\delta_{\text{abs}}(x_i, x_j) = \delta_{\text{abs}}(x_j, x_i) \forall x_i, x_j \in X_{\text{abs}}$. 

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