Compactness Score: A Fast Filter Method for Unsupervised Feature Selection

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\begin{abstract}
Along with the flourish of the information age, massive amounts of data are generated day by day. Due to the large-scale and high-dimensional characteristics of these data, it is often difficult to achieve better decision-making in practical applications. Therefore, an efficient big data analytics method is urgently needed. For feature engineering, feature selection seems to be an important research content in which is anticipated to select “excellent” features from candidate ones. Different functions can be realized through feature selection, such as dimensionality reduction, model effect improvement, and model performance improvement. In many classification tasks, researchers found that data seem to be usually close to each other if they are from the same class; thus, local compactness is of great importance for the evaluation of a feature. In this manuscript, we propose a fast unsupervised feature selection method, named as, Compactness Score (CSUFS), to select desired features. To demonstrate the efficiency and accuracy, several data sets are chosen with extensive experiments being performed. Later, the effectiveness and superiority of our method are revealed through addressing clustering tasks. Here, the performance is indicated
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by several well-known evaluation metrics, while the efficiency is reflected by the corresponding running time. As revealed by the simulation results, our proposed algorithm seems to be more accurate and efficient compared with existing algorithms.

**Keywords:** Big data analytics, unsupervised feature selection, dimensionality reduction, $k$ nearest neighbor distances.

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1. **Introduction**

In recent years, the problem of big data analytics in machine learning is the key to artificial intelligence research. For different areas, such as computer vision (CV) [1, 2] and pattern recognition (PR) [3, 4], huge amounts of data are generated and the obtained data is prone to be high-dimensional, especially with the flourish of the information era. Whereas in practice, various undesired (i.e., redundant or noisy) data usually exist [5, 6], while the problem of dimensionality disaster will be incurred due to the existence of a huge number of attributes. Besides, we will inevitably face various problems when processing these high-dimensional data, such as long-time consumption and huge storage costs. Thus, the processing of such high-dimensional data has attracted tremendous interests from various scholars and different algorithms are proposed, which are mainly classified into two types, i.e., (1) feature extraction [7, 8, 9] and (2) feature selection [10, 11, 12].

For algorithms belonging to feature extraction, some original features are combined in a certain form to construct new features in order to reduce the dimension. As one of the classic algorithms for feature extraction, the Principal Component Analysis (PCA) algorithm has the property of maximizing the variance. Whereas, such algorithm does not simply select features with large variances, but needs to perform feature transformation on the original features, and the feature set obtained is not a subset of the original features. For practical applications, the feature extraction method lacks meaningful explanations and does not specify which features should be extracted.
For algorithms belonging to the other type, i.e., feature selection, the dimensionality reduction process is usually accomplished through removing some unrepresentative or redundant features, and the final feature set is a subset of the original features. Because this type of algorithm can not only improve the performance of the model, but also enhance the computational efficiency, massive algorithms are proposed recently, and they are generally classified into three subcategories, i.e., supervised [13, 14], semi-supervised [15, 16] and unsupervised [17, 18, 19], depending on the extent of label information being used. For the supervised and semi-supervised methods, their performance is mainly affected by the extent of available label information. However, in practice, we usually do not have any label information for the obtained high-dimensional data and labeling such data is usually expensive and time-consuming. Therefore, feature selection algorithms belonging to the unsupervised category are usually most popular and this research is the focus of scholars’ attention [20, 21, 22, 23, 24]. During the past decades, such unsupervised algorithms have significantly facilitated the solving of various classification and clustering tasks [25, 26, 27].

In this manuscript, we devote our efforts to further improving the accuracy and efficiency of unsupervised feature selection methods. Nowadays, from tasks related with high-dimensional data, we find that the local structure seems to be of greater importance than the global structure. In addition, the data are often closer to each other if belonging to the same class. Therefore, the features with more compact internal structures should be selected in order to achieve better clustering effects. Considering this fact, a fast filter method for unsupervised feature selection, Compactness Score (CSUFS), is proposed. An evaluation metric, i.e., Compactness score, is given to reflect the importance of a feature, while $k$ nearest neighbors of a sample are determined to improve performance and simplify the feature selection process. Moreover, an optimized methodology through ordering features is also presented to further reduce the computational complexity. Aiming to evaluate the performance, extensive simulations are performed on several practical data sets and corresponding performance is compared with those of several existing algorithms. As indicated, our proposed
algorithm is illustrated to be accurate in dealing with clustering tasks with reduced computational complexity being reflected by short simulation time. The main contributions of this manuscript are summarized as:

- Considering the fact that data from the same class usually possess compact internal structures, a fast unsupervised feature selection algorithm is proposed.

- To reduce the complexity of determining the sum of $k$ nearest neighbor distances for each sample, we further optimize the feature selection process through making the samples in each feature orderly.

- Aiming to assess corresponding performance of our algorithm, several data sets are selected with extensive experiments being conducted. Corresponding performance is compared with those of several existing algorithms.

Summing up, the overall architecture of our manuscript is provided as: Section 2 presents some existing related works addressing the problem of feature selection. Then, the proposed methodology is briefly provided in Section 3. Following that, several data sets are selected for further analyses while extensive experiments are conducted through the adoption of different algorithms. Corresponding performance is evaluated through comparing the obtained simulation results in Section 4. Eventually, we conclude the manuscript in Section 5.

2. Related works

For unsupervised feature selection method, label information is unnecessary to be required for corresponding analyses; thus, as afore-stated, the investigation of this type of methods has become a hot topic. During the past years, various scholars have devoted their endless efforts to the study of unsupervised feature selection while different algorithms are proposed. For feature selection from the unsupervised perspective, we are anticipated to determine an appropriate subset of features that are capable of maintaining the most discriminative information
while preserving the intrinsic geometric structures at the same time. Generally speaking, the algorithms related to unsupervised feature selection are usually classified into three sub-types, being listed as filter \cite{28, 29}, wrapper \cite{30, 31} and embedded \cite{32, 33}, respectively.

For methods belonging to the wrapper type, the feature selection is deemed as an optimization of searching process, while the subset of features is determined according to the capability of a particular classifier. Through introducing the Support Vector Machines (SVMs) into the wrapper method, Guyon et al. \cite{34} conducted the combinatorial search and the optimum feature subsets is also meliorated. Later, Maldonado and Weber \cite{35} proposed an improved feature selection approach through the adoption of SVMs with kernel functions; thus, the redundant features can be removed efficiently. Additionally, Dy and Brodley \cite{36} developed an enhanced algorithm based on the expectation-maximization clustering, while the performance of identifying possible feature subsets is also investigated through two different evaluation metrics, being listed as scatter separability and maximum likelihood. Due to the features selected by this type of methods are more suitable for pre-defined learning tasks, the wrapper methods tend to be better in terms of performance. However, as mentioned in \cite{18} and \cite{37}, these wrapper methods are usually of high computational costs, and may not be the proper options to deal with high-dimensional data.

For the embedded methods, the feature selection process is usually integrated with the learner training process. This is due to the fact that during the learner training process, feature selection is conducted automatically. For instance, Maugis et al. \cite{38} considered the relationship between irrelevant and clustering variables, while the feature selection process is regarded as a clustering task on the basis of model. Afterwards, Cai et al. \cite{39} proposed a multi-cluster algorithm based on manifold learning, whereas the redundant features are not able to be addressed accordingly. Zhao et al. \cite{40} developed a novel feature selection algorithm from the perspective of spectral in order to identify the redundant features through a sparse multi-output regression. Nevertheless, the performance of this algorithm might be deteriorated due to the conduction of
spectral regression after manifold learning. Later, the authors in [41] developed an unsupervised spectral feature selection algorithm through coevolving of the manifold learning and regression, while a joint model were also presented [18] in order to improve the robustness of selecting features, whereas this algorithm might be unable to depict the fundamental local structure because of the adoption of a predetermined radial basis kernel function. Aiming to characterize data, Du and Shen [42] proposed an advanced structure to select features iteratively instead of utilizing all the features. Nevertheless, this type of method is prone to overfitting, and regularization needs to be introduced to prevent this phenomenon. In addition, only models that can get the coefficient of features or the importance of features have the ability to perform feature selection during the learning process simultaneously.

As to the filter methods, a weight should be assigned to the feature of each dimension with the value indicating the relative importance of the feature of that dimension; this is referred to as feature scoring. According to corresponding scores, features are anticipated to be sorted, while the desired feature subset is composed of the top-ranked features. For instance, maximizing variance is the simplest filter method. It uses unsupervised evaluation indicator variance to reflect the representativeness of features and selects features with large variance. Although this method can select some representative features, it may not be able to distinguish data in different classes. Then, He et al. [43] observed that data are usually close to each other if coming from the same class. Based on this observation, a new standard named Laplacian Score was defined, and this newly-defined score was able to describe the power of locality preserving of features. On the basis of the spectral graph theory, Zhao and Liu [14] proposed an integrated framework to select features through supervised and unsupervised approaches. Through an agglomerative hierarchical means, Liu et al. [44] regarded the feature selection process as feature clustering on the basis of information measurement. Yang et al. [45] developed an integrated mechanism through combining discriminative analysis and $\ell_{2,1}$-norm minimization simultaneously. Additionally, Tabakhi et al. [46] presented an unsupervised feature
selection algorithm to calculate the similarity between features by incorporating the ant colony optimization.

Unlike the afore-mentioned wrapper and embedded methods, feature selection for the filter-based methods does not involve any learning processes. The score of each feature is derived through multiple iterations, and the optimal feature subset is finally obtained according to the ranking of scores. Because both the wrapper and embedded methods consider learning models, corresponding performance is usually much better than filter methods. However, the computational cost of these methods is high, which hinders their use in large-scale data. Therefore, in practical applications, especially for data possessing huge amounts of features, the filter methods are simple and high-efficiency. Nevertheless, for some of the previous filter methods, they may not be able to choose the most representative features and corresponding performance for a specific learning task may be unsatisfactory. In this paper, we mainly devote our efforts to the investigation of the filter methods and propose an improved unsupervised feature selection algorithm for the purpose of further reducing the computational complexity.

3. Methodology

Here, we present the proposed unsupervised feature selection method, i.e., CSUFS, in detail. For each feature, a metric Compactness score is defined in order to evaluate the compactness of the internal structure. Then, the important features are selected by comparing the Compactness score of each feature. Eventually, we also proposed an optimized methodology in order to further simplify the computational complexity.

Before further analysis, we introduce some notations that are utilized throughout this paper. All uppercase bold letters represent matrices, while the lowercase bold letters indicates the vectors, and the lowercase letters without bold denotes scalar values. Let the input data set be depicted as \( X = [x_1, x_2, \cdots, x_n]^T \in \mathbb{R}^{n \times m} \), where \( x_i \in \mathbb{R}^{m \times 1} \) denotes the \( i \)-th sample. For certain sample \( x_i \), cor-
respective $\ell_p$-norm is calculated as:

$$\|x_i\|_p = \left(\sum_{j=1}^{m} |x_{ij}|^p\right)^{\frac{1}{p}}$$  \hspace{1cm} (1)

where $x_{ij}$ indicates the $j$-th feature of the sample $x_i$ and $|x_{ij}|$ denotes the absolute value of $x_{ij}$. Obviously, $\|x_i\|_2$ denotes the $\ell_2$-norm of $x_i$. Alternatively, $X$ is denoted as $X = [f_1, f_2, \cdots, f_m] \in \mathbb{R}^{n \times m}$, where $f_i \in \mathbb{R}^{n \times 1}$ denotes the $i$-th feature and $f_{ij}$ indicates the $j$-th sample of $f_i$.

### 3.1. Proposed method

According to the feature selection theory, there usually exists a low-dimensional data set, which is obtained through removing some unimportant or redundant features from the high-dimensional data set. Our proposed algorithm, i.e., CSUFS, is aiming to obtain such a low-dimensional data set that is capable of improving the computational efficiency as well as the performance, and the details of Compactness Score are illustrated as follows.

The data preprocessing, i.e., normalization, is performed on each sample before conducting the feature selection. Here, preprocessing a sample $x_i$ from $X$ is presented for an illustration: Normalization of $x_i$ indicates that corresponding $\ell_2$-norm should equal to 1, i.e., $\|x_i\|_2 = 1$. Then the $j$-th element of $x_i$, i.e., $x_{ij}$, is provided as:

$$\frac{x_{ij}}{\|x_i\|_2} \rightarrow x_{ij}$$  \hspace{1cm} (2)

Note that $\|x_i\|_2$ in Eq. (2) indicates the $\ell_2$-norm of $x_i$ before normalization.

Then, we are supposed to select a feature from $X$. Here, the $r$-th feature $f_r = [f_{r1}, f_{r2}, \cdots, f_{rn}]^T$ is chosen for an illustration. First, for the $i$-th sample of $f_r$, i.e., $f_{ri}$, we assume the distance from another sample $f_{rj}$ is denoted as $|f_{ri} - f_{rj}|$. Afterwards, we need to find the $k$ smallest distances which indicate the $k$ nearest neighbors for $f_{ri}$. Specifically, the neighbors of $f_{ri}$ can be defined as the samples close to $f_{ri}$ in the feature $f_r$. We define the sum of $k$ nearest
neighbor distances of all samples in the $r$-th feature as $d_r$, which can be obtained as:

$$d_r = \sum_{i=1}^{n} \sum_{j \in V} |f_{ri} - f_{rj}|$$

(3)

where $V$ is the $k$-nearest neighboring set of $f_{ri}$. Through minimizing $d_r$, we can obtain more representative features that have stronger local compactness. After traversing all the features in $X$, a vector $d$ can be determined.

If the samples in a feature are the same, i.e., variance of the feature is close to 0, then this feature is of no use for distinguishing the samples. Variance is utilized to indicate the level of divergence of the samples. Hence, we prefer representative features with relatively large variances. For the selected feature $f_r$, corresponding variance is denoted as $v_r$, which is provided as:

$$v_r = \frac{1}{n} \sum_{i=1}^{n} (f_{ri} - \mu_r)^2$$

(4)

where $\mu_r$ represents the mean of $f_r$, i.e., $\mu_r = \frac{1}{n} \sum_{i=1}^{n} f_{ri}$. Similarly, after traversing all the features, a vector $v$ can be determined.

Here, we define that $Cs_r$ represents the Compactness score of $f_r$, which is calculated as:

$$Cs_r = \frac{d_r}{v_r} = \frac{\sum_{i=1}^{n} \sum_{j \in V} |f_{ri} - f_{rj}|}{\frac{1}{n} \sum_{i=1}^{n} (f_{ri} - \mu_r)^2}$$

(5)

After determining the Compactness scores for all the features, a vector $s$ can be identified. According to the above analysis, we expect to get the few features with the smallest scores. In addition, we assume that the low-dimensional data set is represented as $W = [f'_1, f'_2, \ldots, f'_d] \in \mathbb{R}^{n \times d}$, where $W$ is a subset of $X$; here, $d$ represents the reduced number of features, where $d \ll m$. Therefore, an unsupervised feature selection algorithm for obtaining the optimal solution $W$, i.e., CSUFS, is provided as in Algorithm 1.
Algorithm 1: The CSUFS algorithm.

Input:

Input data set $X = [f_1, f_2, \cdots, f_m] \in \mathbb{R}^{n \times m}$;
Number of selected features $d$;
Number of the nearest neighbors for each sample $k$;

Output:

Low dimensional data set $W \in \mathbb{R}^{n \times d}$.

1. Initialization: $d$, $v$, $s$ are set to be $m$-dimensional zero vectors.
2. Normalize all samples in $X$ to ensure that the $\ell_2$-norm of each sample equals to 1.
3. for $r = 1$ to $m$
   4. Take the $r$-th feature $f_r \in \mathbb{R}^{n \times 1}$.
   5. Update $d_r \in d$ via Eq. (3).
   6. Update $v_r \in v$ via Eq. (4).
   7. Update $Cs_r \in s$ via Eq. (5).
8. Sort the elements in $s$ in ascending order, and record corresponding index values.
9. Take the features corresponding to the first $d$ index values which constitute the desired low dimensional data set $W$. 


3.2. Optimized Compactness Score

When solving Eq. (3), for certain sample $f_{ri}$, the traditional calculation method first needs to compute the distances between it and all the other samples in the same feature. Let $ds_j$ denote the distance between samples which can be computed as:

$$ds_j = |f_{ri} - f_{rj}|$$ (6)

where the value of $j$ is from 1 to $n$, but $j$ cannot be equal to $i$. By calculating the above method in a loop, we can get $n - 1$ distances. Then, these distances need to be sorted in descending order. Among these distances, the first $k$ smallest values are selected, while the summation result is the sum of $k$ nearest neighbor distances of the known sample.

After analysis, the computational complexity of calculating $dr$ in Eq. (3) with the traditional calculation method is $O(n^2 + n^2\log n)$, where $n$ denotes the number of samples. Obviously, the computational complexity is proportional to the number of samples. As long as the number of samples is large enough, the traditional calculation method is suffering from the drawback of time-consuming, which incurs a high computational complexity. To further improve the computational efficiency, we propose an optimized methodology to optimize the process of determining the sum of $k$ nearest neighbor distances.

Before computing $dr$, we first sort the elements in $f_r$ in a certain order (either descending or ascending) to ensure that it is an ordered vector. For the simulations here, we adopt the descending order. Then, we can find that, for each sample, its $k$ nearest neighbors are in its vicinity. In this way, we only need to compute the distance between the known sample and any other sample from the neighboring set, which consists of $2k$ elements at most, i.e., $k$ samples before and $k$ samples after the target one. Here, the reason why $2k$ is adopted is to avoid neighboring samples are all on one side. Therefore, we can compute $ds_j$ with the below method:
\[ d_{s_j} = \begin{cases} 
 f_{r_i} - f_{r_j} & i < j \leq i + k \\
 f_{r_j} - f_{r_i} & i - k \leq j < i 
\end{cases} \] (7)

By the above method, for a certain sample, we can obtain \(2k\) distances and the \(k\) smallest distances are identified accordingly. This method is extremely useful for the samples at both ends of the vector, because their \(k\) nearest neighbors are the following \(k\) samples or the previous \(k\) samples. For the other samples, it is necessary to compute at most the distance between it and the previous \(k\) samples and the following \(k\) samples. Generally speaking, \(k\) is much smaller than \(n\). Therefore, the iterative processes of determining the distances between the target sample and all the other samples can be greatly reduced. After optimization, the computational complexity of calculating \(dr\) in Eq. (3) becomes \(O(kn + kn\log k)\). Compared with the traditional calculation method, the computational efficiency is obviously improved.

As shown in Fig. 1, the elements in the rectangle represent the samples in the feature (here, integers are chosen to simplify the description). The red rectangle represents the selected sample, and the line connection indicates that in order to find the sum of \(k\) nearest neighbor distances, the distance between these two samples needs to be obtained. The number on the connecting line indicates the distance between the two samples. The distance drawn by the red circle represents the final required distance. Here, the value of \(k\) is selected as 2. After comparing the two methods in Fig. 1, the optimized calculation method only requires 4 distances in order to determine the summation of \(k\) nearest neighbor distances, whereas the traditional calculation method requires 9 distances. For simplicity, only ten samples are selected in this example. For practical applications, the number of samples is usually large, whereas \(k\) is small.

In addition, we provide another example aiming to understand the entire process after optimization intuitively as in Fig. 2, where only a small part of the ALLAML data set is selected for simplicity. As indicated, the total number of distances required to calculate the sum of \(k\) nearest neighbor distances of the sample through the optimized calculation method is reduced by a large extent,
Section 3.3. Computational complexity

We know that the efficiency of an algorithm is largely affected by the computational complexity, while in this subsection, we devote our efforts to discussing the computational complexity of the traditional calculation method and the optimized calculation method, respectively.

For the proposed methodology utilizing the traditional calculation method,
for each sample in a feature, we are anticipated to derive the distances between it and all the other ones. The computational complexity of this process is $O(n^2)$. In addition, we also need to obtain the sum of $k$ nearest distances for each target sample; hence, we need to sort all the distances, and select the first $k$ smallest distances. Here, we adopt the Quicksort method [17], which possesses a computational complexity of $O(n \log n)$. Thus, the corresponding computational complexity of conducting the above process for those $n$ samples in the feature is derived as $O(n^2 \log n)$. Besides, the computational complexity of calculating the variance of an $n$-dimensional vector is $O(n)$. Therefore, the computational complexity required to figure out the Compactness score $Cs_r$ of a feature with the traditional calculation method is provided as $O(n^2 + n^2 \log n + n)$. After figuring out all the $Cs_r$, we need to sort them in ascending order. In view of the above analysis, the corresponding computational complexity is derived as $O(mn^2 + mn^2 \log n + mn + m \log m)$.

Nevertheless, as afore-stated, calculating Eq. (3) using the traditional calculation method is time-consuming. Later, we try to analyze the computational complexity of the method after optimization. Instead of solving Eq. (3) directly, we first sort the samples in the feature $f_r$. The complexity is obtained as $O(n \log n)$. Through analysis, to solving Eq. (3), the complexity of adopting the optimized calculation method is obtained as $O(n(k + k \log k))$, i.e., $O(nk + nk \log k)$. The following processes are the same as those in Algorithm 1; hence, the corresponding computational complexity of Optimized Compactness Score is derived as $O(mn \log n + mnk + mnk \log k + mn + m \log m)$. Due to the fact that $k \ll n$, we can say that the corresponding complexity of the optimized method is approximately $O(mn \log n + mn + m \log m)$. Accordingly, we can conclude that the corresponding computational complexity of Optimized Compactness Score is far less than that of Compactness Score utilizing the traditional calculation method.
4. Experimental analysis

In order to validate corresponding efficiency and accuracy, extensive simulations are performed. Several benchmark data sets are selected for illustrations through the application of various feature selection algorithms. Then, simulation results are provided with extensive analyses. Later, aiming to reflect the computational efficiency, corresponding running time is then compared with those of several baseline algorithms when different data sets are considered.

4.1. Data sets

In this manuscript, nine data sets, including four biological data sets (i.e., ALLAML, Leukemia, Lymphoma, Lung), one handwritten digit data set (i.e., MNIST), two face image data sets (i.e., WarpAR10P, Orlraws10P), two other general data sets (i.e., YEAST, BRAIN) are selected for further analyses. All these data sets were downloaded from different websites, such as UCI Machine Learning Repository\(^1\) and scikit-feature feature selection repository\(^2\). Table 1 illustrates the characteristics of selected data sets.

| Data sets  | Samples | Features | Classes |
|------------|---------|----------|---------|
| ALLAML     | 72      | 7129     | 2       |
| Leukemia   | 72      | 7070     | 2       |
| Lymphoma   | 96      | 4026     | 9       |
| Lung       | 203     | 3312     | 5       |
| MNIST      | 3495    | 784      | 10      |
| WarpAR10P  | 130     | 2400     | 10      |
| Orlraws10P | 100     | 10304    | 10      |
| YEAST      | 1484    | 1470     | 10      |
| BRAIN      | 42      | 5597     | 5       |

\(^1\)https://archive.ics.uci.edu/ml/datasets.php
\(^2\)https://jundongl.github.io/scikit-feature/datasets.html
4.2. Existing algorithms

To illustrate the superiority of the proposed algorithm in addressing feature selection tasks, corresponding performance is compared with those of several existed unsupervised feature selection algorithms, which are provided as:

- **All Features (All Fea)**: All features of the data sets are retained in the experiments.

- **Max Variance (Max Var)**: Compute the variance of each feature, then sort the features in a descending order according to the variance magnitude, finally the top few features are chosen.

- **Laplacian Score (LS) [43]**: Compute the Laplacian score of each feature, then features are sorted in an ascending order based on the obtained Laplacian scores, and finally take the first few features with small scores.

- **Unsupervised Discriminate Feature Selection (UDFS) [45]**: Given that the class label of input data can be predicted by a linear classifier, unsupervised feature selection is performed by combining discriminative analysis and $\ell_2,1$-norm minimization into a joint mechanism.

- **Unsupervised Feature Selection with Ordinal Locality (UFSOL) [48]**: In order to preserve the topology information in the neighborhood of each sample, a triplet-based loss function is adopted to select features for distance-based clustering tasks.

- **Uncorrelated Regression with Adaptive graph for unsupervised Feature Selection (URAFS) [49]**: Due to the generalized uncorrelated constraint, generalized uncorrelated regression model (GURM), is proposed to find uncorrelated but discriminative features for unsupervised feature selection.

4.3. Evaluation metrics

Aiming to evaluate the performance of all algorithms, corresponding selected features obtained through different baselines are utilized to deal with the typ-
ical clustering task where K-means is applied. Following related studies on clustering, the clustering performance is evaluated by comparing the obtained labels with those of the original data set. When evaluating the clustering performance of an algorithm, we adopt two evaluation metrics, i.e., clustering accuracy (ACC) and normalized mutual information (NMI).

**Clustering accuracy (ACC):** Let $s_i$ represent the $i$-th original label, and $r_i$ represent the $i$-th label obtained after clustering. Then, ACC is calculated as:

$$ACC = \frac{\sum_{i=1}^{n} \delta(s_i, \text{map}(r_i))}{n}$$

where $n$ denotes the number of samples. Here, $\delta(s, r)$ represents the delta function, which equals to 1 if $s = r$, otherwise it equals to 0. map($r_i$) is a permutation mapping function, which is utilized to map each label obtained through clustering $r_i$ to an equivalent label in the data set.

**Normalized mutual information (NMI):** Let $s$ denote the entire label set of the data set, while $r$ denotes the label set obtained after clustering with the application of our algorithm. The mutual information metric (MI), which refers to the degree of correlation between two random variables, is given as:

$$MI(s, r) = \sum_{s_i \in s} \sum_{r_i \in r} p(s_i, r_i) \cdot \log \frac{p(s_i, r_i)}{p(s_i) \cdot p(r_i)}$$

where $p(s_i)$ and $p(r_i)$ indicate the probability of selecting $s_i$ and $r_i$ from the original label set $s$ and the experimental label set $r$, respectively, and $p(s_i, r_i)$ denotes the joint probability that $s_i$ is selected from $s$, at the same time $r_i$ is selected from $r$.

For the analyses here, NMI is adopted as the evaluation standard which is provided as:

$$NMI(s, r) = \frac{MI(s, r)}{\max(H(s), H(r))}$$

where $H(s)$ and $H(r)$ are the entropies of $s$ and $r$, respectively. Here, $MI(s, r)$ can be determined through Eq. (9). From Eq. (10), we can clearly conclude
that $NMI(s,r)$ varies from 0 to 1. If the two label sets are similar, then the corresponding NMI is close to 1. This shows that the performance of the algorithm is well. On the contrary, if the performance of the algorithm is poor, NMI is close to 0.

4.4. Experimental settings and parameter sensitivity

To evaluate the performances, experiments are performed on a typical clustering task, i.e., K-means clustering. To minimize the effect of random initialization, for each algorithm, we conduct the K-means clustering task for ten times from different starting points and the average results are determined accordingly. Although the ten K-means clustering initializations in an algorithm are different, in order to make the results comparable, we set these ten different initialization processes to be consistent in each algorithm. Two evaluation metrics, i.e., ACC and NMI, are adopted to reflect corresponding performance. Additionally, before performing the clustering task, we normalize the selected nine data sets, which not only improves the computational efficiency, but also avoids the influence of abnormal samples on the results.

After analysis, it is found that there is only one important parameter in Compactness Score, that is, the number of neighbors $k$. ACC is employed to evaluate its clustering performance under different values. The number of selected features are respectively selected from $\{20, 40, 60, 80, 100, 120, 140, 160, 180, 200\}$, while the value of $k$ varies in $\{5, 10, 15, 20, 25, 30\}$. For brevity, we only demonstrate the experimental results on three data sets. The difference in performance under different values is shown in Fig. 5. The results on different data sets show that Compactness Score is robust to $k$ to some extent.

4.5. Results and analysis

Given the selected data sets and baselines, extensive experiments are conducted in this section. Corresponding simulation results of different algorithms are provided in Table 2 and Table 3 respectively. For each value in the tables,
Table 2: ACC(\%) for different selected algorithms on selected data sets.

| Data sets | ALLAML | Leukemia | Lymphoma | Lung | MNIST | WarpAR10P | Orlraws10P | YEAST | BRAIN |
|-----------|--------|----------|----------|------|-------|-----------|-----------|-------|-------|
| All Fea   | 65.28  | 65.28    | 53.13    | 64.53| 54.82 | 25.38     | 67.00     | 37.33 | 76.19 |
| Max Var   | 58.46  | 67.55    | 51.23    | 75.37| 51.98 | 28.46     | 67.36     | 35.04 | 75.32 |
| LS        | 63.89  | 70.96    | 56.06    | 74.29| 48.14 | 22.80     | 72.00     | 35.13 | 74.16 |
| UDFS      | 66.67  | 70.96    | 47.44    | 62.43| 51.17 | 34.62     | 82.00     | 37.66 | 68.40 |
| UFSGL     | 60.61  | 65.66    | 46.69    | 60.68| 22.40 | 29.16     | 68.18     | 35.34 | 77.92 |
| URAFS     | 59.47  | 58.33    | 48.30    | 69.55| 53.80 | 27.27     | 73.00     | 36.28 | 72.08 |
| CSUFS     | 96.09  | 77.90    | 65.63    | 80.34| 58.14 | 35.45     | 89.36     | 41.03 | 81.17 |

Table 3: NMI(\%) for different selected algorithms on selected data sets.

| Data sets | ALLAML | Leukemia | Lymphoma | Lung | MNIST | WarpAR10P | Orlraws10P | YEAST | BRAIN |
|-----------|--------|----------|----------|------|-------|-----------|-----------|-------|-------|
| All Fea   | 7.62   | 7.62     | 56.75    | 52.49| 52.30 | 27.48     | 75.86     | 20.22 | 61.82 |
| Max Var   | 8.33   | 10.09    | 54.94    | 53.62| 48.51 | 25.34     | 76.04     | 17.38 | 62.57 |
| LS        | 6.70   | 12.30    | 60.65    | 53.88| 47.05 | 27.06     | 80.10     | 11.80 | 62.46 |
| UDFS      | 7.41   | 8.64     | 46.03    | 50.40| 47.26 | 36.36     | 80.75     | 13.17 | 52.67 |
| UFSGL     | 4.92   | 8.57     | 41.02    | 49.21| 17.68 | 29.44     | 74.74     | 11.20 | 60.95 |
| URAFS     | 2.81   | 7.97     | 49.70    | 53.60| 50.15 | 24.77     | 75.14     | 11.54 | 59.23 |
| CSUFS     | 83.52  | 32.39    | 61.83    | 54.98| 52.22 | 38.91     | 89.13     | 21.95 | 68.26 |

it is obtained through averaging eleven clustering experiments with a different number of features which is utilized to reflect the average performance of different algorithms. The best results are marked in bold.

As indicated, for the experiments conducted, when the performance is evaluated in terms of ACC, our proposed algorithm is always superior compared with the other algorithms, indicated by a larger ACC value. In other words, the performance of our proposed algorithm is shown to be improved by a large extent for some of the clustering tasks, especially on the ALLAML, Leukemia and Orlraws10P data sets. Whereas, if the performance is evaluated in terms of NMI, our proposed algorithm is superior except the experiments conducted on the MNIST data set while the difference of obtained NMIs for All Fea and Compactness Score is neglectable (only 0.08). For such a scenario, although the average performance of our proposed algorithm is the second best compared with the others, the algorithm is still optimal when the number of features is selected within certain range.

To be more intuitive, we also present the simulations in Fig. 3 and Fig.
for the afore-mentioned two metrics, i.e., ACC and NMI, respectively. As illustrated, the number of selected features is marked as the horizontal axis, while the clustering results given the feature number are regarded as the vertical axis. Simulation results for different algorithms are represented by curves in different colors. Subfigures in Fig. 3 or Fig. 4 indicate the results for different data sets.

As illustrated in Fig. 3, the performance of our proposed algorithm, i.e., CSUFS, is proved to be superior compared with any of the other existing state-of-art algorithms when experiments are conducted on ALLAML, Leukemia and Orlraws10P. While for Lymphoma, the proposed algorithm is the best except when the selected feature number equals to 100. For Lung, our proposed algorithm is also the best when the number of features is between 200 and 400 besides 300. While for MNIST, the performance is always better when the number of selected features is between 100 and 180, when the number of selected features equals to 190, the performance of UDFS is the best, while this changes when the number of selected features increases further. Whereas for the other data sets, our proposed algorithm performs better for the majority of the scenarios. Hence, we can come to the conclusion that our proposed algorithm seems to be generally superior for the majority of the experiments conducted compared with the other existing state-of-art algorithms. When the performance of the clustering tasks is evaluated by NMI being presented in Fig. 4 similar conclusions can also be derived.

Furthermore, in order to reflect the effectiveness of the proposed algorithm, the corresponding simulation time required is further provided as in Table 4. As illustrated, the computational efficiency of the All Fea, Max Var and LS algorithms is higher than other algorithms in most cases. In comparison, the time required for our proposed algorithm utilizing the traditional calculation method seems to be several times that of theirs. After optimization, the computational efficiency has been significantly improved, especially on data sets with a large number of samples, such as MNIST and YESAT. Moreover, we found that even though the computational efficiency of the LS algorithm is quite high, it is not
as good as our improved algorithm on data sets with many samples. In addition, we can see that when processing these data sets, compared with All Fea, Max Var and LS, the computational efficiency of our proposed algorithm is not high. However, the simulation time required for UDFS, UFSOL and URAFS is large in several order of magnitudes. While UDFS seems to be the worst algorithm when addressing these data sets.

Hence, we can come to the conclusion that Compactness Score utilizing the traditional calculation method seems to be comparable with Optimized Compactness Score for data sets with a relatively small number of samples. Though the time required by the optimized method is always shorter than that of the
Figure 4: NMI of K-means clustering tasks on nine data sets with different number of features being selected.

Table 4: Efficiency comparison for different selected algorithms over different data sets. The efficiency is reflected by simulation time measured in seconds.

| Data sets | ALLAML | Leukemia | Lymphoma | Lung | MNIST | WarpAR10P | Orlraws10P | YEAST | BRAIN |
|-----------|--------|-----------|----------|------|-------|-----------|-----------|-------|-------|
| All Fea   | 0.102  | 0.113     | 0.119    | 0.181| 2.054 | 0.092     | 0.211     | 0.192 | 0.124 |
| Max Var   | 0.081  | 0.098     | 0.093    | 0.181| 4.512 | 0.138     | 0.491     | 2.964 | 0.069 |
| LS        | 0.137  | 0.171     | 0.134    | 0.262| 20.893| 0.169     | 0.529     | 7.270 | 0.104 |
| UDFS      | 1343.285| 1287.233  | 236.279  | 91.994| 40.936| 43.358    | 2548.927  | 25.594| 674.200|
| UFSOL     | 383.576| 375.737   | 78.308   | 27.077| 5.201 | 14.114    | 784.189   | 7.549 | 232.402|
| URAFS     | 732.417| 717.967   | 237.258  | 68.805| 68.822| 43.348    | 4914.022  | 30.898| 415.173|
| CSUFS     | 1.819  | 1.785     | 1.341    | 5.089 | 255.761| 1.831     | 4.485     | 130.432| 0.689 |
| CSUFS (Optimized) | 1.093  | 1.232     | 0.760    | 2.517 | 7.381 | 0.985     | 1.863     | 6.239 | 0.322 |

traditional method, the difference is not that large. However, for MNIST and YEAST with a lot of samples, we can see that the required simulation time for
Compactness Score utilizing the traditional calculation method is larger than any of the other selected baseline algorithms, this is incurred by the huge number of iterations resulted by a great number of samples. With the adoption of the optimized methodology, the simulation time is reduced by two orders of magnitudes, i.e., 0.03 and 0.0456 times for MNIST and YEAST, respectively. Thus, we can say that our proposed algorithm is sensitive to the number of samples, especially the Compactness Score utilizing the traditional calculation method. Furthermore, through comparing experiments on MNIST and Orlraws10P, one is the data set with the largest number of samples, and the other with the largest number of features, we can also come to the conclusion that the increase in the number of features will not have a great impact on the computational efficiency of our algorithm, while the increase in the number of samples will have a great impact on the computational efficiency of our algorithm. Similar conclusions can be derived when investigating the simulation results in Table 4.

In view of the above analysis, we can draw the conclusion that the features selected by our proposed algorithm are able to perform well in clustering tasks with an acceptable computational efficiency; furthermore, the Optimized Compactness Score is superior to address data sets with a large number of samples.
5. Conclusion

Recently, along with the information age, huge amounts of data are generated which are usually high-dimensional, while valuable information can be obtained through analyzing these high-dimensional data. However, labeling these high-dimensional data is expensive and time-consuming. Therefore, among those algorithms proposed to deal with large-scale data, unsupervised feature selection has attracted extensive interests recently and feature selection is becoming an important research topic. In this paper, a new unsupervised feature selection algorithm, named as Compactness Score, is proposed from a different perspective by selecting features with a more compact local structure to improve various machine learning tasks. To further improve the efficiency, an optimized methodology is also provided.

Afterward, extensive simulations are performed with the corresponding performance being compared with those of existed algorithms. The selected features are utilized to address some typical tasks, such as clustering. As indicated by simulation results, the proposed unsupervised algorithm is proved to be of a computational efficiency to select the features for high-dimensional data. While the features selected by our proposed algorithms are able to perform well in clustering tasks with an acceptable computational efficiency; furthermore, the optimized methodology is superior to address data sets with a large number of samples.

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References

[1] X. Li, M. Chen, F. Nie, Q. Wang, A multiview-based parameter free framework for group detection, in: Thirty-First AAAI Conference on Artificial Intelligence, 2017.

[2] A. Esteva, K. Chou, S. Yeung, N. Naik, A. Madani, A. Mottaghi, Y. Liu, E. Topol, J. Dean, R. Socher, Deep learning-enabled medical computer vision, NPJ digital medicine 4 (1) (2021) 1–9.

[3] J. Song, L. Gao, F. Nie, H. T. Shen, Y. Yan, N. Sebe, Optimized graph learning using partial tags and multiple features for image and video annotation, IEEE Transactions on Image Processing 25 (11) (2016) 4999–5011.

[4] A. Entezami, H. Sarmadi, B. Behkamal, S. Mariani, Big data analytics and structural health monitoring: a statistical pattern recognition-based approach, Sensors 20 (8) (2020) 2328.

[5] M. H. Law, M. A. Figueiredo, A. K. Jain, Simultaneous feature selection and clustering using mixture models, IEEE transactions on pattern analysis and machine intelligence 26 (9) (2004) 1154–1166.

[6] F. Nie, H. Huang, X. Cai, C. Ding, Efficient and robust feature selection via joint $\ell_{2,1}$-norms minimization, Advances in neural information processing systems 23.

[7] J. Mao, A. K. Jain, Artificial neural networks for feature extraction and multivariate data projection, IEEE transactions on neural networks 6 (2) (1995) 296–317.

[8] M. H. Law, A. K. Jain, Incremental nonlinear dimensionality reduction by manifold learning, IEEE transactions on pattern analysis and machine intelligence 28 (3) (2006) 377–391.

[9] K. Kaplan, Y. Kaya, M. Kuncan, M. R. Minaz, H. M. Ertuñç, An improved feature extraction method using texture analysis with lbp for bearing fault diagnosis, Applied Soft Computing 87 (2020) 106019.
[10] O. Şeref, Y.-J. Fan, E. Borenstein, W. A. Chaovalitwongse, Information-theoretic feature selection with discrete $k$-median clustering, Annals of Operations Research 263 (1) (2018) 93–118.

[11] M. Rezaei, I. Cribben, M. Samorani, A clustering-based feature selection method for automatically generated relational attributes, Annals of Operations Research 303 (1) (2021) 233–263.

[12] C. Xiong, W. Qian, Y. Wang, J. Huang, Feature selection based on label distribution and fuzzy mutual information, Information Sciences 574 (2021) 297–319.

[13] J. M. Pena, R. Nilsson, On the complexity of discrete feature selection for optimal classification, IEEE transactions on pattern analysis and machine intelligence 32 (8) (2010) 1517–1522.

[14] Z. Zhao, H. Liu, Spectral feature selection for supervised and unsupervised learning, in: Proceedings of the 24th international conference on Machine learning, 2007, pp. 1151–1157.

[15] Y. Han, Y. Yang, Y. Yan, Z. Ma, N. Sebe, X. Zhou, Semisupervised feature selection via spline regression for video semantic recognition, IEEE Transactions on Neural Networks and Learning Systems 26 (2) (2014) 252–264.

[16] C. Shi, C. Duan, Z. Gu, Q. Tian, G. An, R. Zhao, Semi-supervised feature selection analysis with structured multi-view sparse regularization, Neurocomputing 330 (2019) 412–424.

[17] J. G. Dy, C. E. Brodley, Feature selection for unsupervised learning, Journal of machine learning research 5 (Aug) (2004) 845–889.

[18] X. Zhu, X. Li, S. Zhang, C. Ju, X. Wu, Robust joint graph sparse coding for unsupervised spectral feature selection, IEEE transactions on neural networks and learning systems 28 (6) (2016) 1263–1275.
[19] D. Ding, X. Yang, F. Xia, T. Ma, H. Liu, C. Tang, Unsupervised feature selection via adaptive hypergraph regularized latent representation learning, Neurocomputing 378 (2020) 79–97.

[20] Z. Li, Y. Yang, J. Liu, X. Zhou, H. Lu, Unsupervised feature selection using nonnegative spectral analysis, in: Proceedings of the AAAI conference on artificial intelligence, Vol. 26, 2012.

[21] C. Hou, F. Nie, X. Li, D. Yi, Y. Wu, Joint embedding learning and sparse regression: A framework for unsupervised feature selection, IEEE Transactions on Cybernetics 44 (6) (2013) 793–804.

[22] M. Yuwono, Y. Guo, J. Wall, J. Li, S. West, G. Platt, S. W. Su, Unsupervised feature selection using swarm intelligence and consensus clustering for automatic fault detection and diagnosis in heating ventilation and air conditioning systems, Applied Soft Computing 34 (2015) 402–425.

[23] S. Du, Y. Ma, S. Li, Y. Ma, Robust unsupervised feature selection via matrix factorization, Neurocomputing 241 (2017) 115–127.

[24] C. Tang, X. Zheng, X. Liu, W. Zhang, J. Zhang, J. Xiong, L. Wang, Cross-view locality preserved diversity and consensus learning for multi-view unsupervised feature selection, IEEE Transactions on Knowledge and Data Engineering PP (99) (2021) 1–1.

[25] T. Hancock, H. Mamitsuka, Boosted network classifiers for local feature selection, IEEE Transactions on Neural Networks and Learning Systems 23 (11) (2012) 1767–1778.

[26] C. T. Tran, M. Zhang, P. Andreae, B. Xue, L. T. Bui, Improving performance of classification on incomplete data using feature selection and clustering, Applied Soft Computing 73 (2018) 848–861.

[27] J. Chen, Y. Zeng, Y. Li, G.-B. Huang, Unsupervised feature selection based extreme learning machine for clustering, Neurocomputing 386 (2020) 198–207.
[28] D. Zhang, S. Chen, Z.-H. Zhou, Constraint score: A new filter method for feature selection with pairwise constraints, Pattern Recognition 41 (5) (2008) 1440–1451.

[29] M. A. Ambusaidi, X. He, P. Nanda, Z. Tan, Building an intrusion detection system using a filter-based feature selection algorithm, IEEE transactions on computers 65 (10) (2016) 2986–2998.

[30] A. Wang, N. An, G. Chen, L. Li, G. Alterovitz, Accelerating wrapper-based feature selection with k-nearest-neighbor, Knowledge-Based Systems 83 (2015) 81–91.

[31] M. Mafarja, S. Mirjalili, Whale optimization approaches for wrapper feature selection, Applied Soft Computing 62 (2018) 441–453.

[32] X. Li, H. Zhang, R. Zhang, F. Nie, Discriminative and uncorrelated feature selection with constrained spectral analysis in unsupervised learning, IEEE Transactions on Image Processing 29 (2019) 2139–2149.

[33] F. Nie, W. Zhu, X. Li, Structured graph optimization for unsupervised feature selection, IEEE Transactions on Knowledge and Data Engineering 33 (3) (2019) 1210–1222.

[34] I. Guyon, J. Weston, S. Barnhill, V. Vapnik, Gene selection for cancer classification using support vector machines, Machine learning 46 (1) (2002) 389–422.

[35] S. Maldonado, R. Weber, A wrapper method for feature selection using support vector machines, Information Sciences 179 (13) (2009) 2208–2217.

[36] J. G. Dy, C. E. Brodley, Feature selection for unsupervised learning, Journal of machine learning research 5 (Aug) (2004) 845–889.

[37] R. Kohavi, G. H. John, Wrappers for feature subset selection, Artificial intelligence 97 (1-2) (1997) 273–324.
[38] C. Maugis, G. Celeux, M.-L. Martin-Magniette, Variable selection for clustering with gaussian mixture models, Biometrics 65 (3) (2009) 701–709.

[39] D. Cai, C. Zhang, X. He, Unsupervised feature selection for multi-cluster data, in: Proceedings of the 16th ACM SIGKDD international conference on Knowledge discovery and data mining, 2010, pp. 333–342.

[40] Z. Zhao, L. Wang, H. Liu, Efficient spectral feature selection with minimum redundancy, in: Proceedings of the AAAI Conference on Artificial Intelligence, Vol. 24, 2010.

[41] X. Zhu, X. Wu, W. Ding, S. Zhang, Feature selection by joint graph sparse coding, in: Proceedings of the 2013 SIAM International Conference on Data Mining, SIAM, 2013, pp. 803–811.

[42] L. Du, Y.-D. Shen, Unsupervised feature selection with adaptive structure learning, in: Proceedings of the 21th ACM SIGKDD international conference on knowledge discovery and data mining, 2015, pp. 209–218.

[43] X. He, D. Cai, P. Niyogi, Laplacian score for feature selection, in: Advances in Neural Information Processing Systems, 2005, pp. 507–514.

[44] H. Liu, X. Wu, S. Zhang, Feature selection using hierarchical feature clustering, in: Proceedings of the 20th ACM international conference on Information and knowledge management, 2011, pp. 979–984.

[45] Y. Yang, H. T. Shen, Z. Ma, Z. Huang, X. Zhou, $\ell_{2,1}$-norm regularized discriminative feature selection for unsupervised, in: Twenty-Second International Joint Conference on Artificial Intelligence, 2011.

[46] S. Tabakhi, P. Moradi, F. Akhlaghian, An unsupervised feature selection algorithm based on ant colony optimization, Engineering Applications of Artificial Intelligence 32 (2014) 112–123.

[47] C. A. R. Hoare, Quicksort, The Computer Journal 5 (1) (1962) 10–16.
[48] J. Guo, Y. Guo, X. Kong, R. He, Unsupervised feature selection with ordinal locality, in: 2017 IEEE international conference on multimedia and expo (ICME), IEEE, 2017, pp. 1213–1218.

[49] X. Li, H. Zhang, R. Zhang, Y. Liu, F. Nie, Generalized uncorrelated regression with adaptive graph for unsupervised feature selection, IEEE transactions on neural networks and learning systems 30 (5) (2018) 1587–1595.