Integrating K-means with Quadratic Programming Feature Selection

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Abstract

Several data mining problems are characterized by data in high dimensions. One of the popular ways to reduce the dimensionality of the data is to perform feature selection, i.e, select a subset of relevant and non-redundant features. Recently, Quadratic Programming Feature Selection (QPFS) has been proposed which formulates the feature selection problem as a quadratic program. It has been shown to outperform many of the existing feature selection methods for a variety of applications. Though, better than many existing approaches, the running time complexity of QPFS is cubic in the number of features, which can be quite computationally expensive even for moderately sized datasets.

In this paper we propose a novel method for feature selection by integrating k-means clustering with QPFS. The basic variant of our approach runs k-means to bring down the number of features which need to be passed on to QPFS. We then enhance this idea, wherein we gradually refine the feature space from a very coarse clustering to a fine-grained one, by interleaving steps of QPFS with k-means clustering. Every step of QPFS helps in identifying the clusters of irrelevant features (which can then be thrown away), whereas every step of k-means further refines the clusters which are potentially relevant. We show that our iterative refinement of clusters is guaranteed to converge. We provide bounds on the number of distance computations involved in the k-means algorithm. Further, each QPFS run is now cubic in number of clusters, which can be much smaller than actual number of features. Experiments on eight publicly available datasets show that our approach gives significant computational gains (both in time and memory), over standard QPFS as well as other state of the art feature selection methods, even while improving the overall accuracy.

Keywords: Feature Selection, Support Vector Machine (SVM), Quadratic Programming Feature Selection (QPFS)

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1. Introduction

Many data mining tasks are characterized by data in high dimensions. Directly dealing with such data leads to several problems including high computational costs and overfitting. Dimensionality reduction is used to deal with these problems by bringing down the data to a lower dimensional space. For many scientific applications, each of the dimensions (features) have an inherent meaning and one needs to keep the original features (or a representative subset) around to perform any meaningful analysis on the data [1]. Hence, some of the standard dimensionality reduction techniques such as PCA which transform the original feature space can not be di-

rectly applied. Dimensionality reduction in such scenarios reduces to the problem of feature selection. The goal is to select a subset of features which are relevant and non-redundant. Searching for such an optimal subset is computationally intractable (search space is exponential) [2, 3]. Amongst the current feature selection techniques, filter based methods are more popular because of the possibility of use with alternate classifiers and their reduced computational complexity (like Maximal relevance (MaxRel), Maximal Dependency (MaxDep), minimal-Redundancy-Maximal-Relevance (mRMR) etc.) [4, 5]) [6].

Recently, a new filter based quadratic programming feature selection (QPFS) method [6] has been proposed which has been shown to outperform many other existing feature selection methods. In this approach, a similarity matrix representing the redundancy among the features and a feature relevance vector are computed. These together are fed into a quadratic program to get a ranking on the features. The computation of the similarity matrix requires quadratic time and space in the number of features. Ranking requires cubic time in the number of features. This cubic time complexity can be prohibitively expensive for carrying out feature selection task in many datasets of practical interest. To deal with this problem, Lujan et al. [6] combine Nyström sampling method, which reduces the space and time requirement at the cost of accuracy.

In this paper, we propose a feature selection approach by first clustering the set of features using two-level k-means clustering [7] and then applying QPFS over the cluster representatives (called *Two-level K-Means QPFS*). The key intuition is to identify the redundant sets of features using k-means and use a single representative from each cluster for the ensuing QPFS run. This makes the feature selection task much more scalable since k-means has linear time complexity in the number of points to be clustered. The QPFS run is now cubic only in number of clusters, which typically is much smaller than actual number of features. Our approach is motivated by the work of Chitta and Murty [7], which proposes a two-level k-means algorithm for clustering the set of similar data points and uses it for improving classification accuracy in SVMs. Chitta and Murty [7] show that their approach yields linear time complex-

ity in contrast to standard cubic time complexity for SVM training.

We further enhance our feature selection approach by realizing that instead of simply doing one pass of k-means followed by QPFS, we can run them repeatedly to get better feature clusters. Specifically, we propose a novel method for feature selection by interleaving steps of QPFS with MacQueen's [8] k-means clustering (called *Interleaved K-means QPFS*). We gradually refine the feature space from a very coarse clustering to a fine-grained one. While every step of QPFS helps in identifying the clusters of irrelevant features (i.e. having 0 weights for the representative features), every step of k-means refines the potentially relevant clusters. Clusters of irrelevant features are thrown away after every QPFS step reducing the time requirements. This process is repeated recursively for a fixed number of levels or until each cluster has sufficiently small radius. Each QPFS run is now cubic in the number of clusters (which are much smaller than actual number of features and may be assumed to be constant). We show that our algorithm is guaranteed to converge. Further, we can bound the number of distance computations employed during the k-means algorithm.

We perform extensive evaluation of our proposed approach on eight publicly available benchmark datasets. We compare the performance with standard QPFS as well as other state of the art feature selection methods. Our experiments show that our approach gives significant computational gains (both in time and memory), even while improving the overall accuracy.

In addition to Chitta and Murty [7], there is other prior literature which uses clustering to reduce the dimensionality of the data for classification and related tasks. Examples include Clustering based SVM (CB-SVM) [9], clustering based trees for k-nearest neighbor classification [10] and use of PCA for efficient Gaussian kernel summation [11]. [12] presents a framework for categorizing existing feature selection algorithms and chosing the right algorithm for an application based on data characteristics. To the best of our knowledge, ours is the first work which integrates the use of clustering with existing feature selection methods to boost up their performance. Unlike most previous approaches, which use clustering as a one pass algorithm, our work interleaves steps

of clustering with feature selection, thereby, reaping the advantage of clustering at various levels of granularity. The key contributions of our work can be summarized as follows:

- A novel way to integrate the use of clustering (k-means) with existing feature selection methods (QPFS)

- Bounds on the performance of the proposed algorithm

- An extensive evaluation on eight different publicly available datasets

The rest of the paper is organized as follows: We describe the background for QPFS approach and the two level k-means algorithm in Section 2. Our proposed Two-level k-means QPFS and Interleaved K-Means QPFS approaches are presented in Sections 3 and 4, respectively. Experimental results are described in Section 5. We conclude our work in Section 6.

2. Background

2.1. QPFS [6]

Given a dataset with M features ($f_i, i = 1, ..., M$) and N training instances ($x_i, i = 1, ..., N$) with Class Y labels ($y_i, i = 1, ..., Y$) the standard QPFS formulation [6] is:

$$f(\alpha) = \min_{\alpha} \frac{1}{2} \alpha^T Q \alpha - s^T \alpha$$

Subject to $\qquad \alpha_i \geqslant 0, i = 1, ..., M; \qquad I^T \alpha = 1.$

$$(1)$$

where, α is an M dimensional vector, I is the vector of all ones and Q is an $M \times M$ symmetric positive semi-definite matrix, which represents the redundancy among the features; s is an M size vector representing relevance score of features with respective class labels. In this formulation, the quadratic term captures the dependence between each pair of features, and the linear term captures the relevance between each of the features and the class labels. The task of feature selection involves optimizing the twin goal of selecting features with high relevance and low redundancy. Considering the relative importance of non-redundancy amongst the features and

their relevance, a scalar quantity $\theta \in [0, 1]$ is introduced in the above formulation resulting in [6]:

$$f(\alpha) = \min_{\alpha} \frac{1}{2}(1 - \theta)\alpha^T Q \alpha - \theta s^T \alpha$$

Subject to $\qquad \alpha_i \geqslant 0, i = 1, ..., M; \qquad I^T \alpha = 1.$

$$(2)$$

In the above equation, $\theta = 1$ corresponds to the formulation where only relevance is considered. In this case the QPFS formulation becomes equivalent to Maximum relevance criterion. When θ is set to zero, the formulation considers only non-redundancy among the features, that is, features with low redundancy with the rest of the features are likely to be selected. A reasonable value of θ can be computed using

$$\theta = \bar{q}/(\bar{q} + \bar{m}) \qquad (2a)$$

where, $\bar{q}$ is the mean value of the elements of matrix Q and $\bar{m}$ is the mean value of the elements of vector s. As θ is a scalar, the similarity matrix Q and the feature relevance vector s in (2) can be scaled according to the value of θ, resulting in the equivalent QPFS formulation of Equation (1). The QPFS can be solved by using any of the standard quadratic programming implementations but it raises space and computational time issues. Time complexity of QPFS approach is $O(M^3 + NM^2)$ and space complexity is $O(M^2)$. To handle large scale data, Lujan et al. [6] proposes to combine QPFS with Nyström method by working on subsamples of the data set for faster convergence. This often comes at the cost of trade-off with accuracy. The details are available in [6].

2.2. Similarity Measure

Various measures have been employed to represent similarities among features [13, 3, 14, 2]. Among these, correlation and mutual information (MI) based similarity measures are more popular. The classification accuracy can be improved with MI as it captures nonlinear dependencies between pair of variables unlike correlation coefficient which only measures linear relationship between a pair of variables [15, 6]. The mutual information between a pair of features f_i and f_j can be computed as follows:

$$MI(f_i, f_j) = H(f_i) + H(f_2) - H(f_i, f_2) \qquad (3)$$

where $H(f_i)$ reperents entropy of feature vector f_i and $H(f_i, f_j)$ represents the joint entropy between feature vectors f_i and f_j [16]. Following variant of mutual information can be used as distance metric [16]:

$$d(f_i, f_j) = 1 - \frac{MI(f_i, f_j)}{\max(H(f_i), H(f_j))} \quad (4)$$

2.3. MacQueen's K-Means Algorithm [8]

This is a k-means clustering algorithm which runs in two passes. In the first pass, it chooses first k samples as the initial k centers and assigns each of the remaining $N - k$ samples to the cluster whose center is nearest and updates the centers. In the second pass, each of the N samples is assigned to the clusters whose center is closest and centers are updated. The number of distance computations in the first and second passes are $k(N - k)$ and Nk respectively. Thus, the number of distance computations needed in MacQueen's k-means algorithm is $2Nk - k^2$. This in effect means that the complexity is $O(Nk)$ [7].

2.4. Two-level K-means[7] Algorithm

Recently, a two-level k-means algorithm has been developed using MacQueen's k-means algorithm [7]. This clustering algorithm ensures that radii of the clusters produced is less than a pre-defined threshold τ. The algorithm is outlined below:

Algorithm *Two-level K-means*(D, k, τ)
Input: Data Set D, Initial Number of Clusters k and Radius Threshold τ.
Output: Set of clusters C $(c_1, c_2, \ldots, c_i, \ldots)$ (with radius $r_i \leqslant \tau$) and the set of cluster centers μ.
1. (**level 1:**) Cluster the given set of data points into an arbitarily chosen k' clusters using MacQueen's k-means algorithm.
2. Calculate the radius r_i of ith cluster using $r_i = \max_{x_j \in c_i} d(x_j, c_i)$, where, $d(.,.)$ is the similarity metric.
3. (**level 2:**) If the radius r_i of the cluster c_i is greater than the user defined threshold τ, split it using MacQueen's k-means with the number of clusters set to $(\frac{r_i}{\tau})^M$, where M is the dimension of the data.
4. **return** the set of clusters (C) and corresponding centers (μ) obtained after level 2.

[7] shows that the above two-level k-means algorithm reduces the number of distance calculations as required by the MacQueen's k-means algorithm, while guaranteeing a bound on the clustering error (details below). The difference between the number of distance computations by MacQueen's k-means algorithm and the two-level k-means algorithm follows the inequality:

$$U - \frac{N\alpha^M R}{\tau} \leqslant ND_1 - ND_2 \leqslant U + \frac{k'\alpha^{2M} R}{2\tau} \quad (5)$$

where, ND_1 and ND_2 are the distance computations in MacQueen's k-means algorithm and two-level k-means algorithm respectively,$\alpha \geqslant 0$ is some constant, R is the radius of the ball enclosing all the data points and U is $(k - k')(2N - k - k')$. If $k' \ll k$, then the expected number of distance computations in level 2 is upper bounded by $N\alpha^M R/\tau$. The parameter τ obeys the following inequality:

$$\frac{N\alpha^M R}{U} \leqslant \tau \leqslant R$$

An appropriate choice of τ is obtained using the inequality

$$\max\left(\frac{R}{(k)^{1/M}}, \frac{R}{(2N - k)^{1/M}}\right) \leqslant \tau \leqslant R \quad (6)$$

The clustering error in two-level k-means algorithm is upper bounded by twice the error of optimal clustering [7]. The time complexity of two-level k-means algorithm is $O(Nk)$ and the space complexity is $O(N + k)$ [7]. The detailed analysis of these bounds can be found in [7].

3. Two-level K-means QPFS

Authors in [7] employ two-level k-means clustering for reducing the number of data points for classification using SVM. We use similar idea except that we cluster a set of features instead of the set of data points. We then apply QPFS on representative set of features. Thus, the problem is transformed into the feature space in contrast with their formultaion in the space of data points. Another key distinction is that we need to work with actual features unlike cluster means as in the case of [7]. This is because the

means of feature clusters are abstract points and may not correspond to an actual features over which feature selection could be carried out. Towards this end, we develop two algorithms, the first one by modifying the MacQueen's k-means algorithm and the other one by modifying the two-level k-means algorithm [7] to return cluster representatives (features) in place of cluster means. Each feature is represented as an N-dimensional vector where N denotes the number of training instances (see Section 2.1). The kth component of this vector denotes the value of the feature in the kth data point. The distance metric between a pair features is defined using mutual information as in Equation (4).

In the following sections, M is cardinality of the (feature) space to be clustered. This takes the place of N which is the cardinality of (data) space in the case of Chitta and Murty [7]. Similarly, N denotes the dimensionality of the (feature) space to be clustered. This takes place of n which is the dimensionality of the (data) space in case of Chitta and Murty [7].

3.1. Variant MacQueen's K-means

We propose a variant of MacQueen's K-means algorithm for clustering the features to produce set of clusters with redundant features instead of clustering datapoints. In each iteration of the MacQueen's K-means algorithm, the nearest point from the updated mean is selected as the new center (called the *cluster representative*). Each iteration needs to compute distance from $M - k$ features to k centers and distance from center to nearest feature in its cluster. Thus, each iteration needs $k(M - k) + M$ distance computations. As MacQueen's k-means uses two iterations, the total number of distance computations would be $2Mk - 2k^2 + 2M$. The complexity is thus $O(Mk)$.

3.2. Variant Two-level K-Means(TLKM)

We propose two-level k-Means algorithm (TLKM) by replacing MacQueen's k-means algorithm with its variant in the two-level k-Means algorithm as given in Section 2.4. It is important to note that we are clustering features rather than the data points. TLKM returns the feature clusters along with corresponding representatives. Following the arguments in [7], we

can derive the bounds on number of distance computations for our proposed TLKM algorithm in a similar manner. The only difference is that we have an additional $2M - k^2$ term as explained in Section 2.4 The bounds for difference in the number of distance computations between variant MacQueen's k-means and TLKM is

$$U - M\left(\frac{(\alpha^N + 1)R}{\tau}\right) \leqslant ND_1 - ND_2 \leqslant U + \frac{k'\alpha^{2N}R}{\tau} \tag{7}$$

Here, U is $2(k - k')(M - k - k')$ and other parameters have same definitions as in Equation (5) of Section 2.4. Further, if $k' \ll k$, then the expected number of distance computations in the second level is upper bounded by $M(2 + (\alpha^N + 1)R/\tau)$ and parameter τ obeys the following inequality

$$M\left(\frac{(\alpha^N + 1)R}{U}\right) \leqslant \tau \leqslant R$$

Following [7], for reducing the number of computations in TLKM algoritm, it is necessary that

$$\max\left(\frac{R}{(k)^{1/N}}, \frac{R}{(M - k)^{1/N}}\right) \leqslant \tau \leqslant R \tag{8}$$

OR,

$$\tau \leqslant \min\left(\frac{R}{(k)^{1/N}}, \frac{R}{(M - k)^{1/N}}\right) \leqslant R \tag{9}$$

Following the arguments in [7], it can be shown that the time and space complexities of the modified two-level k-means for clustering features are $O(Mk)$ and $O(M + k)$, respectively.

3.3. Two-level K-Means QPFS (TLKM-QPFS) Algorithm

We are now ready to present the QPFS based feature selection method using TLKM. We named this algorithm TLKM-QPFS, henceforth. We employ TLKM approach to cluster the features in a given dataset followed by a run of QPFS. Algorithm *TLKM-QPFS* illustrates our proposed Two-level k-means QPFS (TLKM-QPFS) approach.

Algorithm *TLKM-QPFS*(FS, k, τ)
Input: Feature Set FS, Initial Number of Clusters k and Radius Threshold τ.

Output: Final representative feature set F (features) in order of their α values.

1. Find the representatives F using TLKM algorithm as defined in Section 3.2
2. Apply QPFS on the cluster representatives F.
3. **return** Ranked F in the order of α

Time and space complexities for TLKM approach in Step 1 are $O(Mk)$ and $O(M + k)$ respectively. In step 2 of Algorithm *TLKM-QPFS*, QPFS approach is used to rank the k cluster representatives (features) obtained in step 1. Time and space complexities for this step are $O(k^3 + Nk^2)$ and $O(k^2)$, respectively. Therefore, the total time and space complexities of the algorithm *TLKM-QPFS* are $O(Mk) + O(k^3 + Nk^2) \sim O(M)$ and $O(M + k) + O(k^2) \sim O(M)$, respectively. It is clear from this analysis that both the time and space complexities of this algorithm are $O(M)$ as $k \ll M$.

4. Interleaved K-Means QPFS (IKM-QPFS)

We now propose a new algorithm by combining the benefits of clustering approach with QPFS. In this proposed algorithm, we strive to refine relevant feature space from coarse to fine-grained clusters to improve accuracy while still preserving some of the computational gains obtained by TLKM-QPFS. Algorithm *TLKM-QPFS* uses k-means to identify cluster of features which are similar to each other (redundant). A representative is chosen for each of the clusters and then fed into QPFS. QPFS in turn returns a ranking on these cluster representatives. Many of the representatives are deemed irrelevant for classification ($\alpha = 0$). Amongst the sets of clusters whose representatives were deemed irrelevant, consider those with cluster radius $r < \tau$. All the features in the these clusters can be considered irrelevant (since the cluster representative was irrelevant and cluster radius is sufficiently small) and can be thrown away. This also gives us an opportunity to further refine the larger clusters($r > \tau$) potentially improving accuracy by identifying a larger subset of relevant features. This process of executing QPFS after initial run of k-means clustering can be repeated recursively. Each run of k-means further refines the relevant sub-clusters whereas each run of QPFS helps in identifying relevant set of features. This leads to the fol-

lowing algorithm for feature selection which we have named Interleaved K-Means QPFS (IKM-QPFS).

4.1. Interleaved K-Means QPFS (IKM-QPFS) Algorithm

To start with, we first employ k-means to find the a set of cluster representatives. These cluster representatives are then fed into QPFS to get feature ranking on them. The cluster with sufficiently small radius ($r < \tau$) need not be refined further and can be directly use for final level of feature selection. Here, we throw away those representatives whose α values are zero(irrelevant for classification). At the same time, clusters with radius greater than τ need to be refined further. This can be done recursively using above steps. In practice, we need to run the recursive splitting of clusters only upto a user defined level. In our approach, we split each cluster into a fixed number (k) of sub-clusters during k-means splitting. The proposed Interleaved K-Means-QPFS algorithm is presented in Algorithm *IKM-QPFS*.

Algorithm *IKM-QPFS*(FS, k, L, τ)
Input: Feature Set FS, Number of Sub-Clusters k that each Cluster is split into, Radius Threshold τ and Number of Interleaved Levels L.
Output: Ordered set of relevant features F
1. Apply variant MacQueen's algorithm to features in FS; Obtain clusters C, cluster representatives f.
2. Apply QPFS on the cluster representatives f and obtain α.
3. $l \leftarrow 1$
4. $F \leftarrow IRR(C, f, \alpha, k, \tau, l, L)$
5. Apply QPFS on F and rank F according to α.
6. **return** F

The sub procedure IRR(Identify Relevant and Refine) is illustrated in Algorithm *IRR*.

Algorithm *IRR*$(C, f, \alpha, k, \tau, l, L)$
Input: Cluster Set C, Cluster representatives f, α obtained by QPFS, Number of Clusters k, Radius Threshold τ, Number of level l, and Maximum Number of Levels L
Output: Final centers F (features) in order of their α values.
1. **for** each cluster $c_i \in C$

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2.     do
3.         find the radius $r_i = \max_{f_j \in c_i} d(f_j, f_i)$;
           $d(.,.)$ is the distance metric.
4.         if ($r_i < \tau$ or $l = L$)
5.             then if ($\alpha_i > 0$)
6.                 then $F = \cup\{f_i\}$
7.         else
8.             Apply variant MacQueen's k-means
               algorithm to features in cluster $c_i$;
               Obtain clusters $C'$, cluster repre-
               sentatives $f'$
9.             Apply QPFS on the cluster cen-
               ters $C'$ and get $\alpha'$.
10.            $l \leftarrow l + 1$
11.            $F' \leftarrow IRR(C', f', \alpha', k, \tau, l)$
12.            $F \leftarrow F \cup \{F'\}$
13.    return $F$
```

In the above algorithm, *if* condition in step 4 checks if the boundary condition has been reached and no more splitting needs to be done (i.e. maximum number of levels L has been reached or $r_i < \tau$). In which case, if the cluster is relevant ($\alpha_i > 0$), then corresponding features are added to the feature set to be returned (step 6). Else, they are discarded. *Else* condition in step 7 goes on to recursively refine the clusters when boundary condition is not yet reached.

The recursive approach for a sub-cluster at i^{th} level can be visualized as follows. In Figure 1, sub-
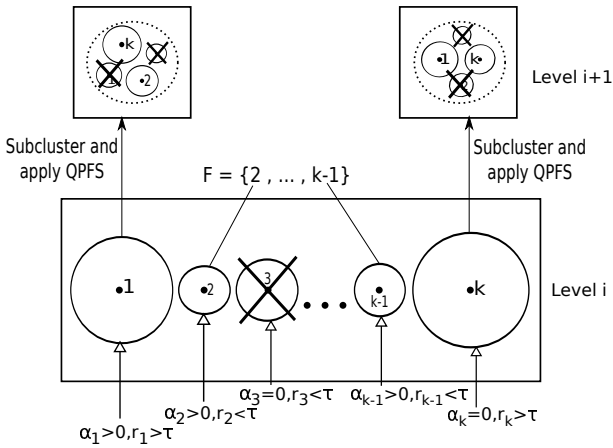

Figure 1: Sub-clustering process at level i

clusters 1 and k have radii greater than τ. They are split further independent of α values. Their contribution to the final feature set is calculated by refining them recursively. Sub-clusters 2, 3 and $k-1$ have radii less than τ. They don't need to be split further. Amongst these, representatives for 2 and $k-1$ contribute to the final set of features. Sub-cluster 3 is discarded since $\alpha_3 = 0$.

4.2. Convergence

In every recursive call of Algorithm *IRR*, all the clusters whose radius is greater than τ are further split into k sub-clusters. Since every split is guaranteed to decrease the size of the original cluster, and we have a finite number of features, the algorithm is guaranteed to terminate and find clusters each of whose radius is less than τ, given sufficiently large L. Note that in the extreme case, a cluster will have only one point in it and hence, its radius will be zero. Now, let us try to analyze what happens in an average case i.e. when the sub-cluster split induced by the MacQueen's algorithm results in uniform-sized clusters. More formally, let r_i denote the radius of the cluster i (at some level) which needs to be split further. Then, the volume enclosed by this cluster is $C * r_i^N$. Here, N is the number of original data points (this is the space in which features are embedded). By the assumption of uniform size, this volume is divided equally amongst all the sub-clusters. Hence, the volume of each sub-cluster is going to be $C * r_i^N / k$. This volume corresponds to a sub-cluster of radius $r_i / k^{1/N}$. Hence, at every level, the cluster radius is reduced by a factor of $k^{1/N}$. If the starting radius is R, then, after l levels the radius of a sub-cluster is given by $R/k^{l/N}$. We would like this quantity to be less than equal to τ. This results in the following bound on l.

$$\frac{R}{k^{\frac{l}{N}}} \leq \tau \implies k^{\frac{l}{N}} \geq \frac{R}{\tau} \implies k^l \geq \left(\frac{R}{\tau}\right)^N$$

$$\implies l \geq N * \log_k\left(\frac{R}{\tau}\right) \text{ (taking log)}$$

Hence, under the assumption of uniform splitting, continuation up to $N * \log_k(R/\tau)$ levels will guarantee that each sub-cluster has radius $\leq \tau$. If $N \approx M$, then features are very sparsely distributed in the data space, and above is a very loose bound. On the other hand if $N \ll M$ (as is the case with many Microarray datasets), then, above bound can be put to practical use.

MacQueen's algorithm starts with the first set of k points as the cluster representatives, followed by another pass of assigning the points to each cluster and then recalculating the cluster representatives. In general, the assumption of uniform sub-cluster may only be an approximation to the actual clusters which are obtained, and hence, above bound will also be an approximation. A detailed analysis of whether one can bound this approximation is proposed to be carried out in future.

4.3. Distance Computations

Distance computations done by interleaved steps of k-means in Algorithm 4 can be bounded as follows. In worst case, none of the clusters will be discarded and also, their radii will be greater than or equal to threshold (τ) at each level. This will lead to recursive splitting of each cluster upto level L. Now, consider cluster c_j at level i. The number of distance computations required by the Mac-Queen's algorithm to split this cluster further is given by $2|c_j|k - 2k^2 + 2|c_j|$ (see Section 3.1). Thus, total number of distance computations at level i is given as $\Sigma_j 2|c_j|k - 2k^2 + 2|c_j| = 2Mk - k^2 + 2M$. The equality follows from the fact that total number of points in clusters at any level is $\Sigma_j |c_j| = M$ (since each cluster is split upto the last level). Therefore, the number of distance computations in worst case is independent of the particular level. Hence, the total number of distance computations for Algorithm 4 can be bounded by $L(2Mk - k^2 + 2M)$.

4.4. Time Complexity Analysis

Time required in step 1 and step 2 of Algorithm *IKM-QPFS* is $O(Mk)$ and $O(k^3)$ respectively. In step 4 of Algorithm *IKM-QPFS*, Algorithm *IRR* is called which is executed recursively. The time required for its execution can be computed as follows:
If the maximum number of levels is L, number of cluster is k then it can be easily shown that the time complexity of Algorithm *IRR* is upper bounded by $O(LMk + k^{3+L})$. The first term comes from the number distance computations in k-means, and the second term comes from the $O(k^L)$ calls to QPFS (k^{i-1} calls at level i), where each call takes $O(k^3)$ time.
Thus, time required in step 4 of Algorithm *IKM-QPFS*

is $O(LMk + k^{3+L})$ and time required in step 5 of Algorithm *IKM-QPFS* is $O(k^{L+3})$.

As L and k are very small constants, total time required by Algorithm *IKM-QPFS* is $O(Mk) + O(k^3) + O(LMk + k^{3+L}) + O(k^{L+3})$ which in effect is $O(M)$.

4.5. Interleaved K-Means Aggressive QPFS (IKMA-QPFS)

In this section, we present a variation on the IKM-QPFS algorithm described above. The key idea is that after every step of QPFS run, we throw away all the clusters whose representatives are deemed irrelevant during a QPFS run (i.e., $\alpha = 0$), independent of the radii of the corresponding clusters. This is a deviation from the original proposed algorithm, wherein, we throw away a cluster only if the corresponding $\alpha = 0$ and the cluster radius $r \leq \tau$. We call this variation Interleaved K-Means Aggressive QPFS (IKMA-QPFS) since it is aggressive about discarding the clusters whose representatives are deemed irrelevant. This potentially leads to even larger gain in terms of computational complexity since IKMA-QPFS tries to identify the irrelevant feature clusters early enough in the process and throws them away. But since some of these clusters can be large in size ($r \geq \tau$), we might trade-off the additional computational gain by a loss in accuracy. But interestingly, in our analysis, we found that almost always this aggressive throwing away of clusters happened only towards the deeper levels of clustering(i.e., very few representatives were deemed irrelevant in the beginning levels of clustering), where the clusters were already sufficiently small. Hence, as we will see in our experiments, not only this variant performs better in terms of computational efficiency than IKM-QPFS, it even simplifies the feature selection problem, giving improved accuracy in some cases.

For IKMA-QPFS, the only change in the Algorithm *IRR* is before step 3 (i.e., right after the `for` loop starts), where we need to put another check `if($\alpha_i = 0$)`. If this condition is satisfied, we simply return out of the function. Rest of the algorithm remains the same. The convergence, the distance computations and the time complexity analyses presented above also remain the same as for IKM-QPFS. This is because all the analyses have been done in the worst

case when no clusters might be thrown away at intermediate levels.

5. Experiments

We compare the performance of our proposed approaches TLKM-QPFS, IKM-QPFS and IKMA-QPFS with QPFS, FGM and GDM on eight publicly available benchmark datasets. We compare all methods for their time and memory requirements and also for their error rates at various numbers of top-k features selected. FGM and GDM methods works for binary classification datasets, therefore comparison with FGM and GDM is not carried out for SRBCT multi-class classification datasets. We observe an improved accuracy for FGM and GDM on normalized dataset in range [-1, 1]. Therefore, we normalized all the datasets in range [-1, 1].

We plot the accuracy graphs for varying (1 to 100) the number of top-k features selected for all the datasets except WDBC. For WDBC dataset, we have reported the results up-till 30 top features as this dataset has only 30 features. Next we describe the details of the datasets and our experimental methodology followed by our actual results.

5.1. Datasets

For our experimental study, we have used eight publicly available benchmark datasets used by other researchers for feature selection. The description of these datasets is presented in Table 1. WDBC is breast cancer Wisconsin (diagnostic) dataset, Colon, SRBCT, Lymphoma, Leukemia and RAC datasets are microarray datasets ([6, 17, 3, 18]) and the last two are vision [18, 19] datasets.

5.2. Methodology

WDBC and USPS datasets are divided into 60% and 40% sized splits for training and testing, respectively as in [18]. MNIST dataset is divided in 11,982 training and 1984 testing instances following [19]. The reported results are the average over 100 random splits of the data. The number of samples is very small (less than 100) in microarray datasets, so leave-one-out cross-validation is used for these datasets. We use mutual information as in [6] for redundancy and relevance measures in the experiments. The data

Table 1: Datasets: detailed description

Dataset	No. of Instances	No. of Features	No. of Classes
WDBC	569	30	2
Colon	62	2000	2
SRBCT	63	2308	4
Lymphoma	45	4026	2
Leukemia	72	7129	2
RAC	33	48701	2
MNIST	13966	784	2
USPS	1500	241	2

is discretized using three segments and one standard deviation for computing mutual information as in [6]. For QPFS, the value of scale parameter (θ) is computed using cross-validation from the set of θ values $\{0.0, 0.1, 0.3, 0.5, 0.7, 0.9\}$. The error rates obtained were very similar to the ones obtained using the scale parameter based on Equation (2a). For TLKM-QPFS, we used cross validation to determine the values of expected number of clusters k (to get τ) and for IKM-QPFS and IKMA-QPFS, we used cross validation to determine the good values τ (threshold parameter) and k' (initial number of clusters). Threshold parameter τ is choosen from the set $\{0.70, \ldots, 0.99\}$ with step size of 0.01. k is choosen from the set $\{ 5,...,1000 \}$ with step size of 5 and k' parameter in IKM-QPFS (as well in IKMA-QPFS) is choosen from the set $[3, 150]$.

After feature selection is done, linear SVM (L2-regularized L2-loss support vector classification in primal) [20] is used to train a classifier using the optimal set of features output by QPFS, TLKM-QPFS, IKM-QPFS and IKMA-QPFS methods. FGM and GDM are embedded methods, so accuracy for both of these methods are obtained according to [18, 19]. The experiments were run on a Intel Core^{TM} i7 (3.10 GHz) machine with 8 GB RAM.

We have presented the variation in the error rates on varying the values of τ with a fixed value of initial number of clusters k'=15 in figure 2 and on varying the values of initial number of clusters k' with a fixed value of τ=0.8 in figure 3 for Colon dataset. On
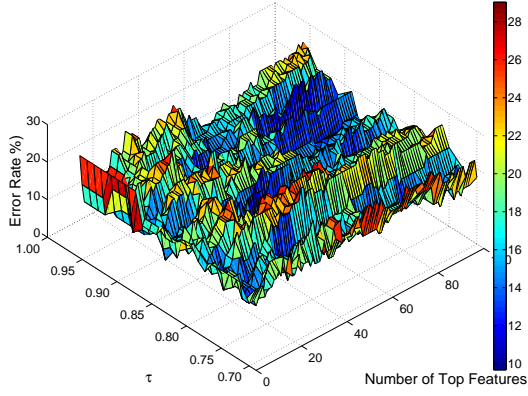
Figure 2: Plot of accuracies (%) for Colon dataset using IKM-QPFS with varying τ and varying number of top $k(1\text{-}100)$ features at fixed initial clusters $k'=15$
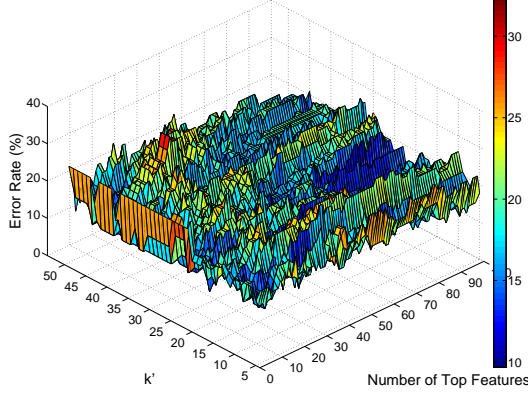

Figure 3: Plot of accuracies (%) for Colon dataset using IKM-QPFS with varying number of initial clusters k' and varying number of top $k(1\text{-}100)$ features at fixed $\tau=0.8$

other datasets, it shows a similar trend.

5.3. Results

5.3.1. Time and Memory

Tables 2 and 3 show the time and memory requirements for feature selection done using each of the methods for all datasets respectively. On all the datasets, TLKM-QPFS,IKM-QPFS and IKMA-QPFS are orders of magnitude faster than QPFS. TLKM-QPFS is three times faster than the GDM on RAC, MNIST and USPS datasets while three to ten times slower than the GDM on WDBC, Colon, Lymphoma and Leukemia datasets. Further, TLKM-QPFS is an order of magnitude faster than the FGM on MNIST

and USPS datasets. IKM-QPFS and IKMA-QPFS are three to five times faster than FGM and GDM on RAC, MNIST and USPS datasets while two to five times slower on WDBC, Colon, Lymphoma and Leukemia datasets. The performance of TLKM-QPFS and IKM-QPFS are comparable while IKMA-QPFS is two to fifteen times faster than TLKM-QPFS and two to six times faster than the IKM-QPFS. This achievement of reduction in time of IKMA-QPFS is due to aggressive throwing of clusters when α becomes zero.

QPFS ran out of memory for RAC dataset in contrast to TLKM-QPFS and IKM-QPFS approaches. Therefore, we use QPFS with Nyström method at Nyström sampling rate $\rho=0.05$ for RAC dataset. The results are appended with $*$ for QPFS with Nyström method in all the tables. For RAC dataset, TLKM-QPFS and IKM-QPFS are more than two orders of magnitude faster than QPFS with Nyström on RAC dataset.

TLKM-QPFS, IKM-QPFS and IKMA-QPFS require more than an order of magnitude less memory compared to QPFS on all the datasets, except MNIST. On MNIST, they require about as much memory as QPFS. The memory required by FGM and GDM are marginally less than TLKM-QPFS, IKM-QPFS and IKMA-QPFS. The memory required by TLKM-QPFS, IKM-QPFS and IKMA-QPFS are comparable on all datasets.

The results in tables 2 and 3, experimentally validates the theoretical complexities for time and memory.

5.3.2. Accuracy

To compare the error rates across various methods, we varied the number of top features to be selected in the range from 1 to 100. For RAC dataset, we varied the number of top features at an interval of 5 in the range from 5 to 100. In tables 4 and 5, $-$ corresponding to a method represents that the experiment was not done with that method. From table 4, it can be observed that our proposed IKMA-QPFS and IKM-QPFS methods achieves lowest error rates for all datasets. In general, IKMA-QPFS and IKM-QPFS achieves lowest error rates earlier than the QPFS for WDBC, SRBCT, Lymphoma, Leukemia and USPS datasets and achieves lowest error rates

Table 2: Comparison of average execution times(in seconds).

Dataset	QPFS	FGM	GDM	TLKM-QPFS	IKM-QPFS	IKMA-QPFS
Colon	104.90	2.04	0.46	**0.44**	1.39	0.76
SRBCT	164.42	-	-	11.65	15.22	**5.91**
Lymphoma	938.73	**0.21**	1.30	32.68	12.41	2.13
Leukemia	4864.69	**0.46**	5.91	17.06	38.35	38.20
RAC	9385.90*	**0.55**	126.82	46.43	31.03	38.89
MNIST	161.69	984.16	268.35	80.37	60.51	**53.28**
USPS	1.34	18.50	3.75	0.84	**0.80**	0.81

Table 3: Comparison of average memory requirements(in KB).

Dataset	QPFS	FGM	GDM	TLKM-QPFS	IKM-QPFS	IKMA-QPFS
WDBC	544	1524	1068	**500**	524	524
Colon	84472	3824	**2472**	9727	10075	9884
SRBCT	100418	-	-	12279	12703	**11231**
Lymphoma	191549	4452	**2936**	14963	12504	10428
Leukemia	636103	10164	**5808**	13874	12503	10427
RAC	1456437*	27284	**17220**	25879	21807	19035
MNIST	97076	253264	**88360**	97111	97111	97111
USPS	40138	14540	**4628**	33435	10394	10394

earlier than FGM and GDM for all datasets except Colon dataset (tables 4 and 5). QPFS achieves lowest error rates earlier than FGM and GDM for WDBC, Colon, Lymphoma and Leukemia datasets. TLKM-QPFS achieves lowest error rates earlier than the FGM for WDBC, Colon, Lymphoma and USPS datasets and also achieves lowest error rates earlier than the GDM for WDBC, Lymphoma and USPS datasets.

Figure 4 plots the error rates for each datasets as the number of top selected features is varied from 1 to 100. The baseline here represents the accuracy obtained when all the features are used for classification and k-means-baseline represents the accuracy obtained when all the representative features (after two-level k-means) are used for classification. It is evident from figures 5.4-5.4 that error rates achieved by TLKM-QPFS, IKM-QPFS and IKMA-QPFS methods are improved over QPFS, FGM and GDM for each of the datasets. In all the datasets, TLKM-QPFS and IKM-QPFS achieve lower error rates with a less

number of top selected features than QPFS. Usually, IKM-QPFS and IKMA-QPFS achieves lower error rates early than the TLKM-QPFS. In figure 4 and figure 5, plots of IKM-QPFS and IKMA-QPFS significantly overlaps.

As expected, the error rates come down as relevant features are added to the set. Once the relevant set has been added, any more additional (irrelevant) features lead to loss in accuracy. Tables 6 and 7 present the average test set error rates for each of the methods for top ranked k features (k being 10, 20, 30,50, 100), where top k features are chosen as output by the respective feature selection method. On all the datasets, IKMA-QPFS performs significantly better than QPFS, FGM and GDM at all the values of top k features selected. Further, error rates for TLKM-QPFS, IKM-QPFS and IKMA-QPFS are comparable on all datasets. This is particularly evident early on i.e. for a smaller number of top-k features. This points to the fact that IKM-QPFS and

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Table 4: Table corresponding to lowest error rates (%)

Dataset	QPFS	FGM	GDM	TLKM-QPFS	IKM-QPFS	IKMA-QPFS
WDBC	3.28	3.49	3.26	3.5	**3.20**	**3.20**
Colon	12.9	11.29	16.13	11.29	9.68	**8.06**
SRBCT	**0.00**	-	-	**0.00**	**0.00**	**0.00**
Lymphoma	**0.00**	2.22	6.67	**0.00**	**0.00**	**0.00**
Leukemia	2.78	11.11	16.67	1.39	**0.00**	**0.00**
RAC	**0.00***	6.06	**0.00**	**0.00**	**0.00**	**0.00**
MNIST	4.13	4.69	4.99	3.83	3.48	**3.43**
USPS	9.02	9.86	10.1	9.49	**8.27**	**8.27**

Table 5: Table for number of features corresponding to lowest error rates (%)

Dataset	QPFS	FGM	GDM	TLKM-QPFS	IKM-QPFS	IKMA-QPFS
WDBC	21	29	25	14	10	10
Colon	5	44	6	14	35	24
SRBCT	11	-	-	9	8	8
Lymphoma	17	47	100	8	7	6
Leukemia	24	37	38	39	34	34
RAC	10*	7	4	9	7	5
MNIST	95	20	75	85	99	99
USPS	93	54	64	34	67	67

IKMA-QPFS are able to rank the relevant set of features right at the top.

TLKM-QPFS performs better than QPFS in all the cases (dataset and number of top k feature combination), except on Colon data at $k = 10$ [3]. Among the two proposed approaches (TLKM-QPFS, IKM-QPFS and IKMA-QPFS), both IKM-QPFS and IKMA-QPFS are clear winner in terms of the accuracy.

5.4. Summary

It is clearly evident from above results that our all the three proposed approaches for feature selection, TLKM-QPFS, IKM-QPFS and IKMA-QPFS, give significant gains in computational requirements (both time and memory), even while improving the overall accuracy in all cases when compared with

QPFS and significantly low error rates when compared with FGM and GDM. Especially, our proposed approaches help reach the relevant set of features early on, which is a very important property of a good feature selection method. The computational requirements of TLKM-QPFS, IKM-QPFS and IKMA-QPFS are similar to each other. On the large microarray dataset our proposed approaches are faster than the FGM and GDM. As for performance, IKMA-QPFS is a clear winner among the three variants

In tables 6 and 7, TLKM, IKM and IKMA represent TLKM-QPFS, IKM-QPFS and IKMA-QPFS, respectively.
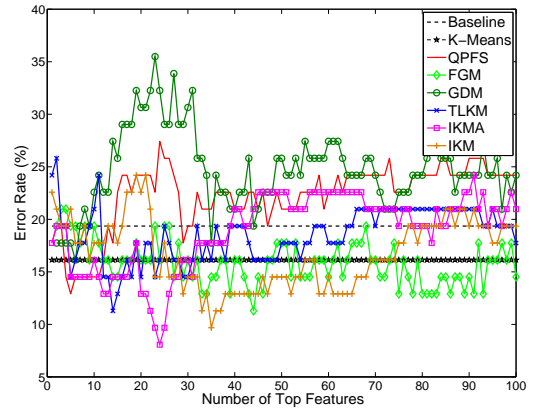
6. Conclusion

In this paper, we proposed an approach for integrating k-means based clustering with Quadratic Programming Feature Selection (QPFS). The key idea involved using k-means to cluster together redundant
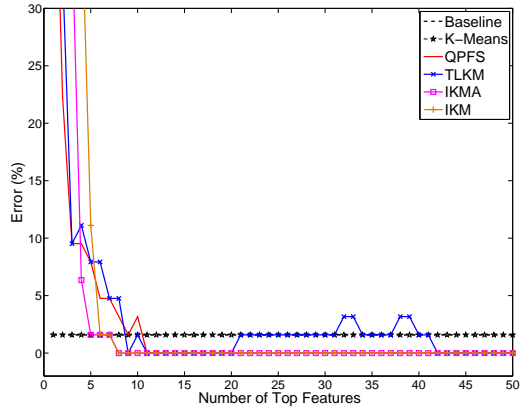

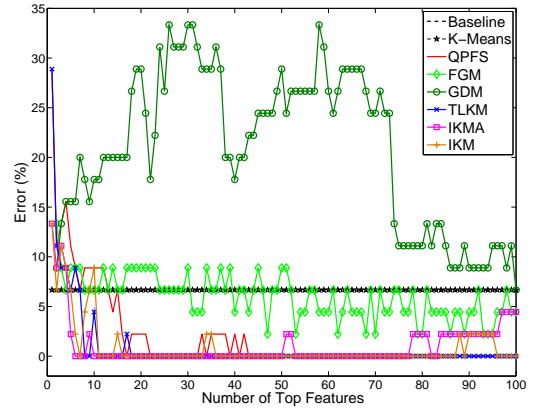[3]it performs marginally worse in couple of cases ($k = 10$, $k = 30$) for SRBCT
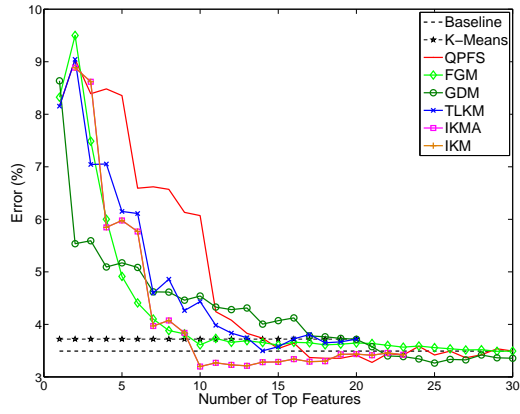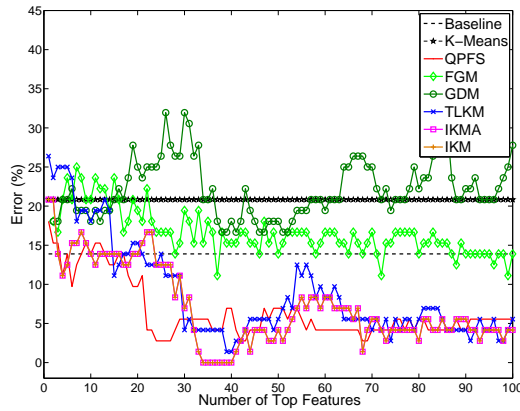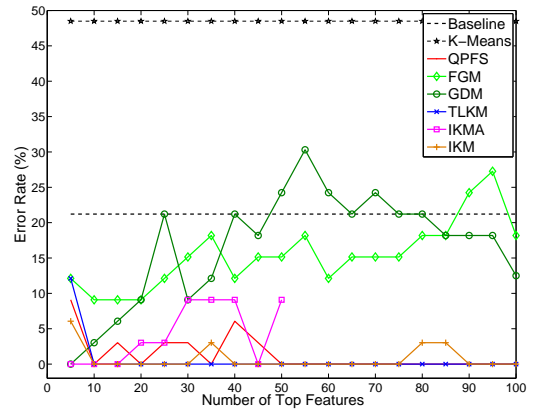
(a) WDBC Dataset

(b) Colon Dataset
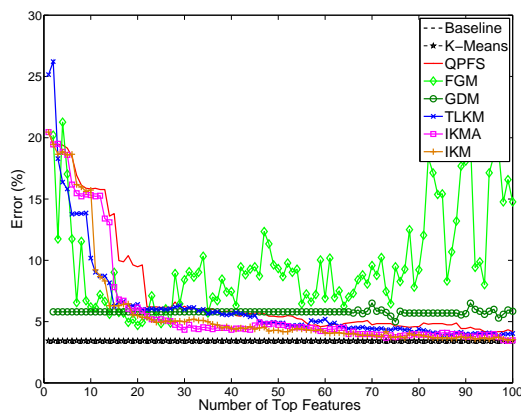
(c) SRBCT Dataset
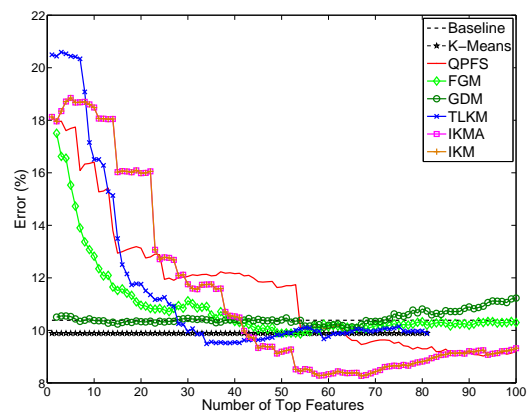
(d) Lymphoma Dataset

(e) Leukemia Dataset

(f) RAC Dataset

Figure 4: Plots of Error rates for each methods with varying number of top k(1-100) features for bioinformatics datesets

(a) MNIST Dataset

(b) USPS Dataset

Figure 5: Plots of Error rates for each methods with varying number of top k(1-100) features for vision datasets

sets of features. Only one representative from each cluster needed to be considered during the QPFS run for feature selection, reducing the complexity of QPFS from cubic in number of features to cubic in number of clusters (which is much smaller). We presented two variations of our approach. TLKM-QPFS used two level k-means to identify a set of representative features followed by a run of QPFS. In the more sophisticated variant, IKMA-QPFS, we interleaved the steps of k-means with QPFS, leading to a very fine grained selection of relevant features. Extensive evaluation on eight publicly available datasets showed the superior performance of our approach relative to existing state of the art feature selection methods.

One of the key directions for future work involves providing a generic framework for integrating a given clustering algorithm with a filter based feature selection method. Other direction includes extending our approach to sparse representations to deal with data in very high dimensions (millions of features, such as in vision). A third direction deals with coming up with a parallel formulation of our proposed approach.

Acknowledgment

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Table 6: Error rates (%) for bioinformatics datasets by each methods

Dataset		k (number of top features)				
		10	**20**	**30**	**50**	**100**
WDBC	QPFS	6.07	**3.41**	3.49	-	-
	FGM	3.61	3.64	3.49	-	-
	GDM	4.54	3.72	3.36	-	-
	TLKM	4.43	3.72	-	-	-
	IKM	**3.20**	3.43	-	-	-
	IKMA	**3.20**	3.43	-	-	-
Colon	QPFS	**14.52**	24.19	19.36	20.97	24.19
	FGM	19.36	16.13	16.13	17.74	**14.52**
	GDM	22.58	30.65	30.65	25.81	24.19
	TLKM	20.97	14.52	**14.52**	17.74	17.74
	IKM	17.74	22.58	**14.52**	**14.52**	19.35
	IKMA	16.13	**12.90**	16.13	22.58	20.97
SRBCT	QPFS	3.18	0.00	0.00	0.00	0.00
	FGM	-	-	-	-	-
	GDM	-	-	-	-	-
	TLKM	1.59	0.00	1.59	0.00	0.00
	IKM	0.00	0.00	0.00	0.00	0.00
	IKMA	0.00	0.00	0.00	0.00	1.59
Lymphoma	QPFS	8.89	2.22	0.00	0.00	0.00
	FGM	6.67	8.89	8.89	8.89	4.44
	GDM	17.78	28.89	33.33	28.89	6.67
	TLKM	4.44	0.00	0.00	0.00	0.00
	IKM	8.89	0.00	0.00	0.00	0.00
	IKMA	0.00	0.00	0.00	0.00	4.44
Leukemia	QPFS	**13.89**	**9.72**	5.56	6.94	5.56
	FGM	20.83	19.44	19.44	13.85	13.89
	GDM	18.06	25.00	31.94	18.06	27.78
	TLKM	18.06	15.28	**4.17**	5.56	5.56
	IKM	**13.89**	13.89	6.94	**4.17**	**4.17**
	IKMA	**13.89**	13.89	6.94	**4.17**	**4.17**
RAC	QPFS+Nys	0.00	0.00	3.03	0.00	0.00
	FGM	9.09	9.09	15.15	15.15	18.18
	GDM	3.03	9.09	9.09	24.24	12.5
	TLKM	0.00	0.00	0.00	0.00	0.00
	IKM	0.00	0.00	0.00	0.00	0.00
	IKMA	0.00	3.03	9.09	9.09	-

Table 7: Error rates (%) for vision datasets by each methods

Dataset		k (number of top features)				
		10	**20**	**30**	**50**	**100**
MNIST	QPFS	15.83	9.47	6.25	5.40	4.83
	FGM	6.20	**4.69**	8.42	9.32	14.77
	GDM	**5.79**	5.79	5.79	5.79	5.85
	TLKM	10.18	6.40	5.99	4.89	4.03
	IKM	15.73	5.50	4.99	**4.3**	3.53
	IKMA	15.32	6.15	**4.33**	4.74	**3.48**
USPS	QPFS	16.41	13.13	12.06	11.65	**9.20**
	FGM	12.82	10.96	11.13	9.89	10.30
	GDM	**10.37**	**10.33**	10.45	10.39	11.23
	TLKM	16.51	11.76	**9.96**	9.83	9.89
	IKM	18.49	15.99	11.76	**9.20**	9.32
	IKMA	18.48	15.98	11.76	**9.20**	9.32

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Abstract

Keywords:

1.