Feature space transformations and model selection to improve the performance of classifiers

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Abstract

Improving the performance of classifiers is the realm of prototype selection and kernel transformations. Prototype selection has been used to reduce the space complexity of k-Nearest Neighbors classifiers and to improve its accuracy, and kernel transformations enhanced the performance of linear classifiers by converting a non-linear separable problem into a linear one in the transformed space. Our proposal combines, in a model selection scheme, these transformations with classic algorithms such as Naive Bayes and k-Nearest Neighbors to produce a competitive classifier. We analyzed our approach on different classification problems and compared it to state-of-the-art classifiers. The results show that the methodology proposed is competitive, obtaining the lowest rank among the classifiers being compared.

Keywords: Learning systems, Kernel methods, Hyper-parameter optimization, K nearest neighbors

1. Introduction

The complexity of classification problems has been continuously increasing due to the availability of more and diverse sources of information. The more detailed characterization of the data along with the amount of information, impose challenges for information processing techniques to remain competitive. Prototype selection approaches aim to reduce the number of examples taking a subset of elements that describe the properties of the complete database, or by generating elements that summarize the available information, see [40]. Both selection and generation of prototypes can be seen as sampling methods that...
retrieve points from a distribution. On the other hand, techniques for feature selection deal with the problem of selecting and generating relevant features that correctly describe all element’s classes of the database, see [39]. Both approaches can be understood as the selection of rows (elements) or columns (features) in a matrix of samples. However, even though creating lower-dimensional data implies less memory and computing resources; the elimination of high correlated features and elements does not always result in better classification accuracy. At this point kernel-based methods come to play; the use of a kernel function is not oriented to achieve dimension reduction, and its objective is to project data into a new feature space where the problem can be easily classified.

Traditionally, the effects of kernel-based transformation and prototype generation and selection are studied separately. This contribution address this research gap by proposing a classification strategy based on projecting the original space into a transformed one using a set of prototypes and a kernel function. Algorithms used for prototypes selection and generation were inspired in the works related to Nyström method; these are a random selection, means, and completing the Furthest First Transversal algorithm. Commonly used kernel functions are incorporated in the approach as well as traditional classifiers such as k-Nearest Neighbors and Naive Bayes. Finally, these components are included in a model selection scheme to decide the combination of prototype method, kernel, and classifier that produces a competitive classification pipeline.

The model selection is performed using the random search on the space formed with the different algorithms; and, the performance is obtained using a k-fold cross-validation approach. Furthermore, the computational cost of performing the random search is exploited with the creation of an ensemble; this ensemble outperforms the base classifiers.

Our approach is analyzed on nine standard benchmarks. Firstly, we examined whether the random search produces competitive classification pipelines; this procedure is compared against grid search. Secondly, the ensemble is contrasted with a single classifier, as expected, the ensemble outperforms the classifier in all the problems. We validate our methodology by performing an extensive comparison with state-of-the-art methods using nine standard benchmarks. The results indicate that our approach is competitive with state-of-the-art techniques.

This manuscript is organized as follows. Section 2 reviews the related work; Section 3 introduces the fundamentals of kernel-based methods, the kernel trick, and the \( k \) nearest neighbors classifier. Our approach is described in Section 4. Section 5, the results, and a comparison with other states of the art classifiers are carried out. Finally, some conclusions and future research directions are given in Section 6.

2. Related Work

Kernel methods have been proved to be useful to improve many machine learning approaches, some examples are: fisher discriminant [28, 27], Support Vectors Machines [41, 17, 38], manifold learning [7, 5, 3], more recently with
Non-parametric density estimation based classifier [37] and even though as Neural Networks activation function [36]. These methods depend on a kernel function, many times represented as a similarity/distance matrix \( K = X^T X \) for a linear kernel), which is given by the kernelized dot product of each element in the dataset. Since computing \( K \) for a large matrix is expensive, in terms of computing time and memory, much research has been done to avoid full computation and storage of \( K \). A common approach to overcome the cost associated to \( K \) is to create the approximation matrix \( \tilde{K} \), where the Nyström method altogether with different sampling procedures for column selection are a widely used strategy [9, 21, 10]. Nyström approximation stands that it is possible to apply any kernel method over \( \tilde{K} \) with little impact on the quality of the result [43]. This approach is mainly oriented to efficiently get a fixed number of eigenvectors [10], due to these methods are often linked to Singular Value Decomposition (SVD), Principal Component Analysis, and QR factorization. In the literature, there are many sampling methods inspired by Nyström approximation, which ranges from random sampling [43], distributional [9], Ridge Leverage Score [31], among others. Kumar et al. [23] provide a comprehensive survey into the field. The state-of-the-art sampling strategy for Nyström method is described at [44, 45], it is based on the usage of K-Means algorithm for computing column’s centroids; centroids are then used as references to map original data to \( \tilde{K} \). Further analysis and improvements of the K-Means method are reported at [18, 42] where authors determined the K-Means is optimal regarding \( || K - \tilde{K} || \) as error function.

In the same line of finding an approximation for \( K \) Coifman and Lafon [7] avoid using all columns by applying the incomplete Cholesky decomposition to select the \( k \) most relevant columns; then, these columns are used to create a low-rank matrix \( \tilde{K} \) where Kernelized Principal Components Analysis (KPCA) was performed. Similarly, Baudat and Anouar [2] state the column selection as an optimization problem. The training set, \( X \), is expressed as a linear combination of the subset of columns \( \hat{X} \subset X \); \( \hat{X} \) is created by using columns that minimize the normalized Euclidean distance between each column vector \( x_i \) and its projection by using \( R \) and a weights vector \( w \), where the number of features vectors, as well as their weights, must be determined. Lui and Zio [26] describe a further modification to apply this approach to regression problems; the authors formulate the problem as a least-squared error optimization problem with equality of constraints. The hyper-parameters are optimized with Grid Search [11], that is, evaluating a grid of pre-established parameter values.

On the other hand, prototype selection algorithms tackle the problem of large datasets by reducing the number of items in a dataset. Further, a carefully selected set of prototypes can also improve the overall performance of a classification task. Perhaps the most basic representative of this family of methods is the Nearest Centroid (NC) classifier. This method computes one centroid per class, i.e., through the geometric dimension mean. The classification procedure is pretty simple, that is, the class of a non-labeled exemplar is computed as the class of its nearest centroid [22]. Despite its simplicity, NC is powerful enough to be used in many applications, mainly for text catego-
rization, due to its simplicity, efficiency, and its proved performance on text classification [6]. Nonetheless, prototype selection algorithms many times, target k-Nearest Neighbor algorithms instead of NC.

We can found multiple methods for prototype generation in literature. In [25], an optimization method, inspired by the gravitational model, is used to determine a weighted mass factor for each prototype; this method is especially useful for imbalanced data sets. In [24], the initial centroids are optimized by minimizing the hypothesis margin under the structural risk minimization principle; and finally, the kernel method is used to deal with linear inseparability in the original feature space. All the above techniques are applied mainly to text classification, to the best of our knowledge, there are not centroid based classifiers that tackle general classification problems.

A generalization of the center-based classifier can be seen as cluster-based classifier where more than one centroid per class is chosen, many examples of this kind of approaches come from prototype selection. According with [40], the most widely used algorithms of this type that present the best results in their respective publications are: Self-generating prototypes (SGP) [14], Reduced Space Partition (RSP) [35] and Pairwise Opposite Class-nearest neighbor (POC-NN) [33]. All methods mentioned above aim to split the dataset in a set of clusters where elements at each cluster are homogeneous, i.e., all of them belong to the same class, by always using class boundaries elements; therefore, the main difference among these methods is how elements are selected. For instance, SGP uses hyperplanes and singular value decomposition, while RSP selects the furthest elements at each non-homogeneous cluster. In the case of POC-NN, the cluster division is led by POC-NN prototypes which are used as locations for setting separating hyperplanes. De Brabanter et al. [8] propose an alternative algorithm for prototype selection based on the approximation of the kernel matrix; authors select a subset of the elements that maximize the quadratic Rényi entropy criterion. This algorithm is oriented to optimize fixed-size least squares support vector machines, introduced in [38].

Our approach is similar to prototype selection since a set of references are generated; these references can be computed as either centroids, i.e., elements are created by summarizing elements at each group; or centers, i.e., prototypes that are already in $X$. The precise strategy depends on the problem. Nonetheless, the main difference with other state-of-the-art approaches is that references are selected in an unsupervised manner. Note that this strategy may also suffer from different problems, like the lack of local support for creating a decision function. In this article, we use different strategies to tackle this problem based on clustering and the k-center problem [16]. In this road, a clustering algorithm based on compactness of the space is required, since the proposed methodology borrows the idea of clustering based prototype’s selection and kernel methods to generate a new feature space (not necessarily linear separable) where simple classifiers like k-Nearest Neighbors (kNN) and Naïve Bayes (NB) might achieve competitive performance. For our scheme, we use kNN classifier since it is based on similarity (and dissimilarity) measurements, and this is the core of kernel methods. Additionally, we include NB because the new feature space
may promote the independence of variables. Nevertheless, there is no restriction to use other classifiers instead of the $k$NN and NB.

Moreover, the set of references are no used to train a classifier directly; instead, they are used to project original data to a new feature space with the help of a kernel function. Our proposal is highly related to Nyström’s K-Means sampling, and the central differences are that Nyström methods are usually applied to approximate the top $k$ eigenvalues to perform features reduction (since it is column-wise), while our method aims to locate border references for a classification task, as our method is row-wise. Moreover, most of Nyström methods sample directly from $K$, whereas our approach samples over the original data. Additionally, our method recognizes that many parameters are highly dependent on the classification task, so we state our problem as a model selection problem that finds a competitive classifier among a large set of possible ones. The following section is dedicated to detail our contribution.

3. Kernel Methods

Kernel-based methods have been widely used in industrial-strength applications due to its excellent performance. The idea behind a kernel method is to transform the shape of the feature space from some distribution to another one that simplifies the classification task. For example, consider a linear classifier, capable of performing an accurate classification if the data is linearly separable like that illustrated in Figure 1(a), the classifier only needs to distinguish between items on the left and right of the dividing hyperplane. On the other hand, if the dataset cannot be linearly separated, like Figure 1(b), then a linear classifier fails in finding a good performing model for the data. Instead of discarding the linear classifier, an option is to transform the shape of the dataset using a kernel function (maybe a non-linear one) such that a hyperplane can perform a proper division of the classes, perhaps projecting the input dataset into a lower or higher dimension space, for example, Figure 1(c) shows a projection of data in Figure 1(b) in space where a linear separation can be achieved.

3.1. Kernel trick and $k$NN

Usually, kernel methods map a set of features to a new space by using the so-called kernel trick. Any algorithm can take advantage of the kernel trick whenever it can be expressed in terms of a dot product [29]; this situation is typical for classification algorithms. Therefore, the following formulation defines the mapping:

$$\psi(x) : \mathbb{R}^m \rightarrow \mathbb{R}^m'$$

The kernel trick takes advantage of the fact that a dot product evaluates to a scalar value, changing the problem of finding $\psi$ to a more convenient function $\phi : \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R}$, such that:

$$\phi(x_i, x_j) = \psi(x_i)^T \cdot \psi(x_j).$$

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(a) An almost linear separable set of points. (b) A non-linearly separable dataset. (c) A linear separable dataset after transforming points in Fig. 1(b).

Figure 1: Example of linear and non-linear separable binary classification problems.

The function given at Eq. 2 is called a kernel [30]. It has the advantage that it works on the original space, so it is not necessary to carry out the explicit mapping.

A simple version of a kernel method classifier can be exemplified by using $k$-Nearest neighbor ($k$NN) method, this is a non-parametric algorithm that uses all known observations of the training set composed by the set of points $X = \{x_i\}$, and its associated set of labels $L = \{\theta_i\}$, to predict outcomes based on a similarity function; $k$NN is flexible enough to work with both similarity and dissimilarity functions. When $k = 1$ the method works as follows. Given a vector $u$, its nearest neighbor $x_i \in X$ is located, then the label $\theta_i$ is associated with $u$. That is, for a dot product similarity, the most similar object is computed as $\arg\max_{1 \leq i \leq |X|} \langle u, x_i \rangle$ or $\arg\min_{1 \leq i \leq |X|} d(u, x_i)$ in the case of a distance function. The latter form gives the name to the method the nearest neighbor of $u$. Many times it is better to use more neighbors to predict; when $k > 1$ the prediction can be computed as the most popular label among $k$ nearest neighbors. The similarity between $u$ and some neighbor $x$ is used to weight the possibility of some label. For instance, the kernelized version of nearest neighbors using the squared Euclidean distance is computed as follows:

$$\text{nn}(u, X) = \arg\min_{1 \leq i \leq |X|} \phi(u - x_i, u - x_i).$$  \hspace{1cm} (3)

Equation 3 can be understood as projecting $u$ in the kernel space given for the dataset $X$ and determining its neighborhood using a linear kernel (i.e. Euclidean Norm). Figure 2 shows the learned decision boundary for a toy example (two concentric circles), for instance. For the classification, a $k$NN classifier with $k = 5$ and uniform weighting is used; we also use the Euclidean distance, the angle between vectors as distance, and the Jensen-Shannon divergence as a distance metric, see [12]. As the figure illustrates, for this particular case, the better option is the Euclidean distance. In any case, the figure exhibits the decision boundary of the kernelized $k$NN. Please notice that the $k$NN algorithm
produces a non-linear decision boundary, even with the application of linear kernels.

![Decision boundaries for kNN with different distance functions](image)

Figure 2: Decision boundaries for $k$NN with different distance functions; yellow points are predicted with light-yellow regions and purple with light-purple regions.

Conveniently, our approach does not reside on the global separation, but in a local-sense of class separation. This strategy helps in solving different kinds of problems without the need for sophisticated kernel functions. Nonetheless, we understand that different kernel functions work better for different problems; therefore, we designed our method to support a relatively small number of kernels, those widely studied and tested from many machine learning approaches [15, 20, 46, 29].

4. A model selection approach for kernel methods

For our purposes, a classifier is a function $h : \mathbb{R}^d \to \mathcal{L}$; that is, $h$ maps a real-valued $d$-dimensional vector to a member of $\mathcal{L}$, which is a set of categorical values. In particular, $h$ is an item among $\mathcal{H}$, the infinite set containing all possible functions with the $h$'s signature. Given a classification task $(X, y, \text{err})$. The idea is to find a function $h \in \mathcal{H}$ that reaches an acceptable error ratio by using a cross-validation scheme. The selection of such $h$ is known as training step. Testing set $X', y'$ is used to validate $h$'s performance; the testing set is no available during the training step.

In this context, $X$ and $X'$ are subsets of $\mathbb{R}^d$, of size $n$ and $m$, respectively; while $y$ and $y'$ are also subsets of $\mathcal{L}^n$ and $\mathcal{L}^m$, respectively. Finally, the function $\text{err} : \mathcal{L}^n \times \mathcal{L}^m \to \mathbb{R}^+$ computes the similarity or fitness between its arguments. Therefore, the training step is the process of finding $h$ such that the function $\text{err}(y, h(X))$ is minimized. For our experiments we measure the Balanced Error Rate (BER) which is defined as the average proportion error, per-class, as follows:

$$\text{BER} = \frac{1}{|\mathcal{L}|} \sum_{c \in \mathcal{L}} \frac{\text{false positives}_c + \text{false negatives}_c}{\#\text{samples}_c}.$$
Since smaller BER values are better than higher ones, we are interested in $h$ functions such as that $\text{err}(y, h(X))$ is minimal.

Our method searches for the parameters $(\phi, R, C)$, where $\phi$ correspond to the kernel, $R$ is the set of references, and $C$ is the classifier, that can prove its competitive performance for the given classification task $(X, y, \text{err})$. These parameters, jointly, define a configuration; the set of all possible configurations is named a configuration space. The tuple $(\phi, R, C)$ is a meta-specification of the configuration space to search for, which in turn represent functions in $\mathcal{H}$. In particular, the selection of these three parts can be tightly linked, and, consequently, these must be selected jointly. Since we use stochastic algorithms to explore the configuration space, it is desirable to produce high-quality predictors of the performance of each configuration; we choose to embed a cross-validation scheme into the $\text{err}$ function.

In summary, we can explain our approach as the following pipeline. Given a training dataset, we select a subset of it based on a distance function and a sampling method (we call this subset as references); the sample is then used, along with a kernel function, to map the original space into a new kernelized space. Afterward, an internal classifier is trained using the kernelized dataset; for instance, we use $k$NN and a Naïve Bayes classifiers. Once the classifier is created, labels of unseen samples can be predicted in a similar way, that is, the references are used along with the distance function and the kernel function to map the original object to the kernelized space; the internal classifier is then used to predict the label of the sample using its mapped representation. The rest of this section is dedicated to detail these parameters.

4.1. Selection of the set of references

We consider four different sampling methods. In any case, we can use samples directly as centers, or we can refine these samples using them as input to compute centroids. We define a center point as an item that is part of the dataset; while a centroid is the geometric mean of a group found by the clustering algorithm. The computation of centroids is straightforward using regions of a Voronoi partition induced by centers. Hereafter, we will use the term references to indicate the use of both centers and centroids.

Random selection. It is a stochastic algorithm based on taking a random sample, evaluate each configuration, and select the best among the sample. More detailed, we select $R \subset X$ randomly; as commented, it is possible to create a set of centroids computing the nearest neighbor in $R$ of each item in $X$; the geometric mean of those items having $c \in R$ has its nearest neighbor produces the centroid associated to $c$’s region. In some sense, random selection copies the input distribution; however, there is no control about how to handle very dense or very sparse regions.

K-means. The set of references is computed employing the K-means clustering algorithm; we use the $kmeans++$ to select initial centroids (seeds) and reduce intra-cluster variance [1]. We only consider centroid references and the Euclidean distance as the dissimilarity measure for this method.
Density Based Clustering. This iterative algorithm starts with an empty $R$ and selects a random item in $c \in X$; the set of $\ell$ nearest neighbors of $c$ in $X$ is removed; the procedure repeats while $|X| > 0$. Each $c$ is added into $R$ to create the set of references. Also, the set of nearest neighbors are used to compute the related centroids. The number of references is $k = \lceil |X|/\ell \rceil$. This approach is related to Density-net construction; the procedure yields to remove most probable regions first, and continues removing $\ell$ items per iteration; the latter iterations capture and remove least probable regions. Uniformly distributed datasets do not have a preference in the capturing order.

Farthest First Traversal (FFT). This algorithm is an approximation of the $k$-centers problem and was simultaneously proposed by [16] and [19]; the approximation of FFT is at most two times the optimal solution. The algorithm selects a set of centers $R$ such all items in $R$ are furthest among them. Since FFT simulates a traversal, each iteration selects an element $c$ as the furthest element from the elements already selected; more detailed, let $r$ be the distant used to select the $i$th element, then a Delone set is formed with the following properties for some distance function $d$:

- All centers are separated by at least $r$, i.e., $d(p, q) > r$ for any pair of centers $p, q \in R$.
- All objects are covered by some center under $r$ radius, i.e., $d(x, c) \leq r$ for $x \in X$ and $c \in R$.

Let us define $d_{\min}(x) = \min\{d(x, c) \mid c \in R_C\}$, that is, the distance between $x$ and its nearest center in $R$; then Algorithm 1 defines the Furthest First Traversal method.

\begin{algorithm}
\textbf{Input:} $X$ a metric database and $k$ the number of centers
\textbf{Output:} the set of $R$ furthest samples
$R \leftarrow c$ where $c$ is selected randomly from $X$
while $|C| < k$ do
    $w \leftarrow \arg \max\{d_{\min}(x) \mid x \in X \setminus R\}$
    $R \leftarrow R \cup \{w\}$
end
\end{algorithm}

Summarizing, FFT chooses $k$ centers such that the maximum distance from some $x \in X$ to its nearest center in $R$ is minimized; at the same time, it maximizes the inter-cluster distance. Centroid references are generated in the same way that in Density Clustering. Please notice that FFT can use any distance function.

4.2. Feature generation

Once the references $R$ are computed, a kernel function $f$ is used to generate the new kernelized feature space $\hat{X}$. More detailed, $f(x, R)$ over each $x_i \in X$; i.e.
\[ \hat{X}_i = f_k(x_i, R) = \{ f(x_i, c_1), \ldots, f(x_i, c_k) \}, \] where \( f(x_i, c_j) \) is the kernel function (similarity or distance \( d \)). For a linear kernel \( f(x_i, c_j) = d(x_i, c_j) \). Table 1 shows four kinds of kernel functions \( f \), which are those used for our experiments; here, \( \sigma \) is set to the maximum intra-cluster distance, i.e., the \( \max_j \{ d(x_{ij}, c_j) \} \), where \( x_{ij} \) is the furthest element from reference \( c_j \) in cluster \( j \). For FFT, we set the last \( r \) values as \( \sigma \); for the rest, each region has its own \( \sigma \) value defined as the maximum distance from an item in the region and its reference. Algorithm 2 describes the feature generation process.

### Table 1: Kernel functions for two vectors \( x \) and \( c \).

| Name   | function                        |
|--------|---------------------------------|
| Linear | \( d(x, c) \)                   |
| Gaussian | \( e^{-d(x, c)/\sigma} \)    |
| Sigmoid | \( \frac{1}{1+e^{-d(x, c)/\sigma}} \) |
| Cauchy | \( \frac{1}{1+d(x, c)/\sigma} \) |

**Input:** \( X \) the metric database, \( k \) the number of features, and \( f_k \) kernel function.

**Output:** \( \hat{X} \) database new features space

\[ R \leftarrow \text{SamplingMethod}(X, k) \]

\[ \hat{X} \leftarrow \{ \} \]

\[ \text{for } x \in X \text{ do} \]

\[ \hat{x}_i = f_k(x, R) \]

\[ \hat{X} \leftarrow \hat{X} \cup \{ \hat{x} \} \]

**end**

**Algorithm 2:** Generation of new feature space

#### 4.3. Internal classifiers

Our approach uses either \( k \)NN or Naïve Bayes as internal classifiers. We select \( k \)NN since it is a well-known non-linear classifier; it is straightforward to use over the new space, and it is a well-known kernel method. It is worth to mention that \( k \)NN uses a distance function to work; we use Euclidean and Angle distances, but any distance function can be used. The selection of the current distance is independent of that used in previous stages. It is possible to use from one to several neighbors to make the decision; also, we can select to use weight each neighbor in a uniform or differently, for example, based on the distance to the sample being processed.

#### 4.4. Hyper-parameter optimization

Once our pipeline is defined; it is necessary to select the precise algorithm for each classification task. As explained in previous sections, we use hyper-parameter optimization to select a competitive classification over a large configuration space; recall that we describe our set of classifiers through its configuration §4. Table 2 summarizes a grid of parameters that define the configuration
space. This grid contains more than ten thousand different configurations; however, some of the possible ones are not valid like those having Naïve Bayes as its internal classifier and varying $k$NN’s parameters. In sum, the configuration space contains close to 4500 valid configurations. Notice that parameters are represented as a set of categorical values since most parameters are categorical indeed.

The model’s performance prediction is computed with a k-folds cross-validation procedure. For instance, our experimental section show results for selecting models using 3-folds. This model validation reduces the chances of a model’s overfitting while ensures the selection of a competitive model due to its precise predictions. The selection is led by the balanced error rate (BER) measure. We dubbed this process, and our classifier itself, as Kernel-based Model Selection (KMS).

While the evaluation of the configuration space can be performed in several ways, we decide to use the low-cost Random Search (RS) meta-heuristic over parameter’s boundaries defined in Table 2. The random search consists of uniformly sampling the configuration space, evaluate the performance of each configuration in the sample, and then select the best performing setup. For instance, our experimental results of the next sections were computed with a sample of 128 configurations. We decide to perform Grid Search (GS) over the configuration space, i.e., an exhaustive evaluation of the complete grid, with the idea of determining an upper bound of Random search over the defined configuration space. The interested reader in these meta-heuristics is referred to [4].

The exploration of the entire space is prohibitive, due to its size and evaluation’s cost for each instance. For instance, each configuration pipeline is evaluated in 4.11 seconds, the time becomes 8.76 minutes for 128 instances for RS and close to six hours for GS. Even when it is possible to reduce this cost with parallel and distributed computation, it is worth to mention that RS

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| Name                          | Value                              |
|-------------------------------|------------------------------------|
| Number of references $k$      | \{4, 8, 16, 32, 64\}               |
| Distance function             | \{Angle, Euclidean\}               |
| Sampling method               | \{Density, FFT, K-Means, Random\}  |
| Kernel function               | \{Linear, Gaussian, Sigmoid, Cauchy\} |
| Reference’s type              | \{Centers, Centroids\}             |
| Internal classifiers          | \{Naïve Bayes, $k$NN\}             |
| $k$NN weighting scheme        | \{Distance, Uniform\}              |
| $k$NN distance function       | \{Angle, Euclidean\}               |
| Number of neighbors           | \{1, 5, 11, 21\}                   |
achieves competitive results and even when it is possible to improve its performance it becomes a simple and effective alternative to other costly methods like GS, and also being susceptible to be optimized for high-performance computing environments. Other meta-heuristics may be of use on more overwhelming combinations.

4.4.1. Improving performance via ensembling

To stabilize and improve the performance, we ensemble a group of KMS instances into a KMS ensemble (KMSE); the ensemble is also used to avoid overfitting since several configurations are harder to overfit. The procedure requires the selection of a group of models having a proved high performance; therefore, we select top-performing classifiers under the random search application. While this procedure keeps the ensembling method simple, we also maintain a construction cost low since the construction time remains almost identical to any of our hyper-heuristic optimization schemes.

In particular, our ensemble implementation uses a voting scheme to determine the label of new samples. A procedure to determine the size of the ensemble is studied in §5.2.1.

5. Experiments and Results

We select to compare and validate our methods using nine benchmarks from the Gunnar Raetsch’s collection.\(^2\) These datasets have been widely used to measure the performance of classification methods in the literature. Each benchmark has 100 training and test splits, except for the image benchmark which has only 20 splits. Table 3 briefly summarizes our benchmarks.

| Benchmark | Dimension | Training | Test |
|-----------|-----------|----------|------|
| banana    | 2         | 400      | 4900 |
| thyroid   | 5         | 140      | 75   |
| diabetes  | 8         | 468      | 300  |
| heart     | 13        | 170      | 100  |
| ringnorm  | 20        | 400      | 7000 |
| twonorm   | 20        | 400      | 7000 |
| german    | 20        | 700      | 300  |
| image     | 20        | 1300     | 1010 |
| waveform  | 21        | 400      | 4600 |

5.1. Performance comparison based on the average BER distribution

In the next paragraphs, we present an experimental comparison of grid search and random search, along with an upper bound performance in §5. Finally,
we provide a rank test that compares our approach with several state-of-the-art classifiers; this test supports our claims regarding the performance of our contribution showing a significant performance improvement in most of our benchmarks as compared with other alternatives.

Figure 3: BER distribution for training and testing sets
Figure 3 shows the average BER distribution for training and testing set over our nine benchmarks. Please recall that each benchmark consists of one hundred random permutations being standard in the literature; therefore, we use the average error over these permutations. Let us start describing our the graphical symbols of this experiment. Purple shapes show the performance distribution over the training set; the green one also shows the performance distribution yet the error, BER, is evaluated over the testing set. In particular, we show the associated histogram and a kernel density estimation for the performance on the training set. The mean of the training distribution is marked with a small inverse triangle on each figure. Finally, we marked the smallest mean of BER for each group of methods with a vertical red line; this line coincides with one of the little triangular ticks. These marks help to visualize the best method for a benchmark based on its average performance.

Figure 3(a) shows the performance distribution for the banana benchmark; we can observe that testing performance is much better than that predicted in training; the best average BER in the training set is achieved by K-Means and closely followed by FFT. When the entire configuration space is considered, it is possible to select any sampling methods since Grid Search (GS) and Random Search (RS) search performs pretty good. Please recall that RS’s cost is a fraction of the GS’s cost. The performance on the testing set shows that almost all methods improve their performance on it, with respect to the training set. This underestimation may indicate that it is possible to learn better for this benchmark; however, it also may indicate significant differences between training and testing sets; Section 5.3 detail more about the performance of other classifiers.

The performance of our methods for thyroid benchmark is depicted in Figure 3(b); contrary to banana, the performance in the testing may achieve better than that predicted in the training set. The average training’s BER is pretty equilibrated among all methods; however, the performance variance is large. The FFT and K-Means perform the better while Density performs the worst. Note that RS has a lower performance than GS; however, RS allows to preserve a competitive average-performance with a lower computational cost.

Figure shows the performance over the diabetis benchmark 3(c). In this dataset, K-Means and Random achieve a bad average BER performance while FFT and Density obtained the best BER values. RS performs slightly better on average than GS.

Figure 3(d) shows the average BER distribution for heart benchmark; here, the mean and the concentration is different among methods. The FFT sampling method performs better than the rest, on average. As in previous benchmarks, GS performs better on average than RS. It is interesting to note the existence of several families of performances inside a configuration space, as several modes can be identified in the BER testing’s distribution; we tackle and also take advantage of this effect through the use of model selection. Notoriously with a small performance footprint due to the effectiveness of RS and GS.

The ringnorm benchmark is compared in Figure 3(e); here, we found that Density-based sampling is much better than others, and FFT performs the worst. In contrast with other benchmarks, RS and GS perform pretty similar;
Table 4: BER performance comparison of different sampling/clustering strategies for the KMS, for both single instance-based and ensemble-based classifiers. The lowest BER is marked in bold.

| Sampling method | banana | thyroid | diabetes | heart | ringnorm | twonorm | german | image | waveform | avg. rank |
|-----------------|--------|---------|----------|-------|----------|---------|--------|-------|----------|----------|
| **Ensemble of size 15 – KMSE** |        |         |          |       |          |         |        |       |          |          |
| Grid Search     | 11.8674 | 5.2540  | 28.5736  | 17.5002 | 2.993    | 2.3935  | 27.6993 | 4.1060 | 9.6862   | 2.8889   |
| Random Search   | 11.8211 | 5.0193  | 28.4153  | 17.4153 | 2.939    | 2.3935  | 27.8255 | 4.1385 | 9.6847   | 2.1111   |
| FFT             | 11.8759 | 5.7095  | 28.3546  | 17.3063 | 2.4197   | 2.3935  | 27.6905 | 4.0160 | 9.6554   | 3.3333   |
| Density         | 11.8082 | 5.7482  | 28.4576  | 17.6550 | 1.5416   | 2.3935  | 27.8255 | 4.0313 | 9.6871   | 4.4444   |
| K-Means         | 11.8650 | 5.5461  | 30.3468  | 17.9031 | 2.1106   | 2.4171  | 30.0933 | 5.4472 | 9.7501   | 7.4444   |

| Single-instance classifier – KMSE |        |         |          |       |          |         |        |       |          |          |
|-----------------------------------|--------|---------|----------|-------|----------|---------|--------|-------|----------|----------|
| Grid Search                       | 12.1121| 6.3542  | 29.1704  | 19.2822| 2.9766   | 2.7716  | 28.5940 | 4.2541 | 10.4001  | 8.2222   |
| Random Search                     | 12.2591| 5.8725  | 28.6336  | 18.0004| 2.8452   | 2.8138  | 28.6013 | 4.1768 | 10.5603  | 8.2222   |
| Density                           | 12.4595| 6.5098  | 28.7612  | 18.4442| 1.8676   | 2.6776  | 28.6285 | 4.2485 | 10.2585  | 8.3333   |
| Grid Search                       | 12.3577| 6.1779  | 29.3124  | 18.6941| 1.8669   | 2.8312  | 28.8386 | 4.3004 | 10.4729  | 9.2222   |
| K-Means                           | 12.3414| 5.9333  | 31.6174  | 18.5642| 2.3011   | 2.6320  | 35.3282 | 5.2402 | 10.4213  | 9.4444   |
| Random Search                     | 12.3804| 6.0724  | 29.8256  | 18.8256| 2.8041   | 2.7609  | 28.6629 | 4.4665 | 10.5185  | 9.5556   |

As RS has a lower cost, its usage is indicated over GS. Figure 3(f) shows the performance for the twonorm benchmark for which we found a uniformity of average performances with a low variance in training and a wider one in the testing set.

On the german benchmark, we found that the K-Means method achieves the lowest performance in both training and testing sets; FFT, Random, and Density perform almost the same. Regarding ensemble methods, RS achieves the best performance slightly surpassing GS. Figure 3(h) illustrates the average BER distribution for the image dataset; here we observe that K-Means, Random selection, and Density-based selection achieve a poor performance. FFT gets the lowest average BER among alternative sampling methods. Again, RS over the performance of GS. Finally, the performance on waveform is uniform, all methods are close regarding average BER on the training set, but best performance is achieved by Density; on the other hand, RS ensemble has a lower mean than GS ensemble.

In summary, we found that different sampling strategies work better for different problems; we cannot say that it is a better general strategy. The evidence may suggest that each problem has particularities such that each method takes advantage differently. This way, even when a particular sampling method performs inadequately, compositional methods like Grid search and Random search remain competitive. In this sense, it is also worth to mention that Random search performs consistently good under our measure, i.e., the mean of the average BER distribution, it is remarkable that Random search may also be faster than Grid search for large configuration spaces.

5.2. The performance of ensemble-based KMSE classifiers

Table 4 shows the average BER for our benchmarks. The selected models are the best ones in the training set using the specified method, and the error is measured in the testing set. The table shows two kinds of values, average BER values, and average rank positions; methods are ordered by the average rank achieved by each method in all benchmarks. Please recall that lower BER
values are better; also, we desire lower average ranks since the best possible rank is 1.

The table lists the performance of both single-instance methods and ensemble methods; ensemble methods listed in the table have fifteen instances under a voting scheme; the 15 instances were selected as the best-performing ones in training set among the evaluated configurations, in either GS or RS. In particular, both RS and GS perform the optimization taking into account all sampling methods while methods listed as a single sampling method perform an RS fixing the sampling method but with the rest of the configuration space expanded. The precise method to determine the size of the ensemble is detailed in the next subsection.

As shown in Table 4, methods based on ensembling consistently outperform single classifiers; please notice that we indicated the separation between single instance classifiers and ensembles in the table, but the rank is not modified. In addition to this natural segmentation, it is possible to see that once we ensembled our KMSE, some sampling methods achieve better performances than its single-instance counterpart regarding the same methods in both single-instance and ensembles. For instance, Random is the worst-performing strategy when a single instance is considered but becomes the fourth better when it is ensembled; a similar effect arises with GS. On the other hand, K-Means does not improve after ensembling as compared with other ensembles. Density-based selection is the third better of single-instance methods and achieves the penultimate position among ensemble methods. RS has a competitive performance in both single-instance and ensemble versions.

The best ensemble method is found with GS, followed by RS. On the third place, we found FFT which achieves five best positions for diabetes, heart, german, image, and waveform. FFT could be the best method, but it has a poor performance on ringnorm. So, here resides the power of GS and RS since both explore the entire set of parameters and can turn around when bad cases arise for a good method. On the rest of the benchmarks, Random selection achieves two best places for banana and ringnorm; Density selection performs the better for ringnorm and GS for thyroid. Please recall that all best places arise on ensemble methods. It is worth no mention that GS obtained just one best place and RS none of them, and both occupy the best positions on the global ranking due to their competitive and low variant performance.

5.2.1. About the size of the ensemble

The purpose of ensembling is to improve and stabilize the expected performance; it is also used to avoid overfitting for a dataset. The ensemble uses the prediction of several single-instance KMS to generate a single prediction based on a majority voting scheme.

Our KMSE includes the selection of top-$\ell$ performing instances, measured in training set. In particular, we use the already evaluated classifiers computed for Random search; therefore, the cost of creating a KMSE is almost identical to that achieved with the Random search method except for Grid search that
evaluates an entire grid of search parameters while explores the configuration space.

Instead of selecting the size of the ensembling based on an additional cross-validation stage, we determine the size using a consensus scheme. In this scenario, the consensus is measured as the agreement in the label’s predictions between a KMSE with top-\(\ell\) instances, and those labels predicted with a KMSE with top-\((\ell + i)\) instances. Figure 4 illustrates the consensus of KMSE on our nine benchmarks; in particular, the figure starts on \(\ell = 3\) and fixes \(i = 2\). Each curve is the proportion of discordant predictions for K-means, FFT, Random selection, and Density-based selection; it also shows Random search that gathers all different sampling methods. All discordant ratios were normalized by the maximum ratio per benchmark to obtain values between 0 and 1.

Figure 4 shows how small values of \(\ell\) produce the most significant differences among predictions. It is worth to mention that prediction’s computational cost is tightly linked to \(\ell\) and we shall select a value that ensures low variance in the predicted labels but also low cost in the prediction procedure. Based on the figure, it is fair to set \(t\) between 9 and 25; these values yield to a consensus with relatively low computing cost. We decided to use \(\ell = 15\) since it has stable consensus in almost all benchmarks; the performance is compared in §5.2 and listed in Table 4 for KMSE models with 15 instances.

5.3. Comparison among different alternatives

Table 5 compares our KMS and KMSE with sixteen classifiers implemented in scikit-learn [32], and two state-of-the-art classifiers, EvoDAG [34] and PSMS [13]; EvoDAG is based on genetic programming and PSMS on particle swarm optimization. As before, we use 15-instance KMSE. Results are ordered by average rank, the best performance among each classification dataset is in boldface to facilitate the reading. Our KMSE gets the better performance on two bench-
Table 5: Comparison of KMS and KMSE with other classifiers

| name          | banana | thyroid | diabetis | heart | ringnorm | twonorm | german | image | waveform | avg. rank |
|---------------|--------|---------|----------|-------|----------|---------|--------|-------|----------|-----------|
| KMS           | 12.25  | 6.12    | 29.34    | 18.69 | 1.87     | 2.83    | 28.89  | 4.30  | 10.47    | 6.00      |
| PSMS          | 11.08  | 6.20    | 27.06    | 20.69 | 7.98     | 3.09    | 30.10  | 2.90  | 12.80    | 5.56      |
| EvoDAG        | 12.77  | 9.13    | 25.46    | 16.6  | 2.66     | 3.11    | 29.8   | 5.17  | 11.48    | 5.56      |
| Gaussian NB   | 11.55  | 11.51   | 28.61    | 10.34 | 1.44     | 2.4     | 30.58  | 3.67  | 12.21    | 7.44      |
| Gradient Boosting | 13.84 | 8.25    | 28.52    | 21.06 | 6.65     | 5.74    | 31.08  | 2.09  | 13.62    | 8.22      |
| MLP           | 19.75  | 9.31    | 28.61    | 14.33 | 16.96    | 2.92    | 32.03  | 3.35  | 11.38    | 8.22      |
| Nearest Centroid | 46.33 | 22.49   | 28.19    | 16.66 | 24.09    | 2.32    | 27.00  | 37.69 | 12.96    | 9.22      |
| AdaBoost      | 28.16  | 8.73    | 29.32    | 22.51 | 7.01     | 5.35    | 31.58  | 3.2   | 14.64    | 10.78     |
| Linear SVM    | 49.97  | 16.91   | 28.47    | 16.8  | 25.18    | 3.58    | 32.44  | 18.65 | 14.2     | 11.22     |
| Logistic Regression | 49.99 | 20.18   | 28.29    | 16.97 | 25.29    | 2.92    | 32.07  | 18.74 | 13.73    | 11.33     |
| Extra Trees   | 13.49  | 6.56    | 32.99    | 21.06 | 8.42     | 7.76    | 36.95  | 2.38  | 16.48    | 11.44     |
| Random Forest | 13.59  | 7.86    | 31.93    | 21.42 | 9.58     | 8.89    | 36.72  | 2.1   | 16.87    | 11.67     |
| K Nearest Neighbors | 11.92 | 12.06   | 32.12    | 18.64 | 43.72    | 3.76    | 36.18  | 5.26  | 13.8     | 12.11     |
| Bernoulli NB  | 41.46  | 32.47   | 33.88    | 16.82 | 28.33    | 5.83    | 32.78  | 39.03 | 14.53    | 14.22     |
| Decision Tree | 15.21  | 9.28    | 33.85    | 27.06 | 19.2     | 20.87   | 36.51  | 3.38  | 20.78    | 14.56     |
| SGD           | 50.28  | 17.69   | 34.03    | 22.19 | 32.65    | 3.89    | 38.5   | 25.12 | 17.61    | 17.00     |
| Passive Aggressive | 49.04 | 19.48   | 34.68    | 23.31 | 31.48    | 3.85    | 38.65  | 26.24 | 17.1     | 17.11     |
| Perceptron    | 56.15  | 18.18   | 34.56    | 21.59 | 33.49    | 3.92    | 37.47  | 26.69 | 19.03    | 17.44     |

marks thyroid, and waveform with an average rank of 3.89; please recall that the best possible average rank is 1. Our single-instance classifier, KMS, is on fourth-position with an average rank of 6.00. EvoDAG shares the second-position with PSMS; and in particular, EvoDAG is the better method for diabetis and PSMS for banana.

Please note that our KMS does not achieve any best position, but it is competitive in all benchmarks so it can be competitive from a global perspective. In contrast, the Gaussian Naïve Bayes achieve the sixth position in the global rank having two best positions (heart and ringnorm); this may indicate high variance in some benchmarks, that for instance, its performance on both banana and image benchmarks is quite low. On the contrary, Bernoulli Naïve Bayes reaches the fifth least performing method. The performance of the kernel-based method Support Vector Machine (SVM) with Radius Basis Kernel (RBF) is pretty good achieving the fifth-best position in the global ranking with an average rank of 7.00. The linear SVM is several positions below with an average rank of 11.22; this behavior is the result of having several non-linear problems among our benchmarks.

Other methods with best-performing classifiers are Gradient Boosting and Nearest Centroid, for image and twonorm respectively. Several of the resting methods achieve pretty good results in some benchmarks but perform pretty bad in others. It is worth to mention that K nearest neighbors method is the sixth least performant method with an average rank of 12.11; this method is the classifier used by our KMS and KMSE without either the machinery for space transformation nor hyper-parameter optimization.

5.4. Analysis of the parameter selection

Table 6 shows a brief analysis of the structural composition of the classifiers over our benchmarks; more precisely, it shows the empirical probability that each parameter is selected to be used by the best classifier using Random search over the configuration space. To compute the top-1 classifier we performed two kinds
of selection, the selection on the training set and selection directly on the test set; the latter scheme is unrealistic, but it is an indicator of the objective distribution of each parameter. The table is divided into several groups, that indicate the parameter being analyzed. There are three columns, and the first indicates the parameter name and two more columns to list the selection’s empirical probabilities.

Regarding sampling algorithms, Table 6 shows that Density achieves the higher selection probabilities; also, FFT and Random selection are almost equally selected. In contrast, K-Means has a low probability to be selected. When the model is selected evaluating on the test set, the probabilities are pretty similar, but FFT is more probable to be selected at the cost of K-Means. Please recall that previous experiments in §5.3 compare and analyze the performance of each sampling algorithm in each benchmark and that our current analysis is over our nine benchmarks. These globally scoped results show that sampling algorithms are useful and they contribute almost equally to tackle our benchmarks efficiently; in particular, K-means is below the usage mean, but it is essential to maintain it as an option since its performance is different from other alternatives and it can be useful for other never-seen benchmarks.

On the distance and kernel functions, we can observe a small variation among alternatives. Regarding distance functions, we observed that both angle’s distance and Euclidean distance have a similar selection probability and that Cauchy kernel and Gaussian are the most selected ones.
The number and kind of references are also analyzed in Table 6. The number of references is forced to be in any of the listed values (i.e., 4, 8, 16, 32, and 64) to simplify the visualization. In general, larger values achieve higher selection probabilities. It is possible to increase the number of references to achieve better results; however, both computational cost and the model’s complexity may suffer from a high number of references.

Regarding the classifier, \(k\)NN classifiers are selected most of the times, more than 70% of the time. However, some problems take advantage of a Naïve Bayes approach; please recall that the classification algorithm is applied in the projected space and that the input space for NB is different than that of the original problem. Finally, when \(k\)NN is selected, the probability of using the angle between vectors as distance function is slightly higher than that of using the Euclidean distance, in both training and testing selection; this is different from the distance function used in the initial stages of our approach where the probability of using both distances are pretty similar and less consistent in training and test selections. The number of neighbors is another parameter where training and testing model selection yield to quite different probabilities; while evaluating in the training set indicate the use of a large number of neighbors, the performance achieved in test suggest the use of 5 and 11 neighbors.

It is worth to notice that our Random Sampling balances the probability of classifiers, and if \(k\)NN is selected, then it proceeds to select other \(k\)NN related parameters. All probabilities are local to the selection, that is, \(k\)NN parameters are accounted only if \(k\)NN becomes the selected classifier.

6. Conclusions

This work proposes two classifiers, KMS and KMSE, based on mapping an input problem into a new space using kernel functions. The idea is that the projected data is simpler to classify with typical \(k\)NN and Naïve Bayes methods. These methods are, in fact, an entire pipeline that allows us to adapt to a wide range of problems, from linear to non-linear tasks. In essence, each classifier produced with our pipeline is composed by a distance function, a sampling method, a kernel function, and a simple classifier working on the mapped space. We experimentally show that each sampling strategy adapts better for different problems; each sampling method is parametrized by the sample size and the kind of object to be sampled, i.e., part of the dataset, or computed and not necessarily being part of the dataset. We call these selected items as references by its duty of projecting the original space into a new one. In a way, these landmark points are used to discriminate locally around them with a boosting improvement from kernel functions.

Also, we ensembled several instances into our KMSE. This ensemble-based classifier improves the performance of the single-instance classifier KMS and performs competitively with state-of-the-art alternatives on our nine benchmarks. Even when the prediction cost is increased proportionally to the ensemble’s size, the construction cost is almost similar to the single-instance KMS. It is necessary to mention that our KMSE uses a simple voting scheme, and more work is
necessary to find better algorithms to summarize individual predictions into a global predicted prediction.

We validated our claims experimentally by using a well-known set of database benchmarks. The results show that our methods are competitive, under average BER, with a wide range of classification methods, including other kernel methods like SVM with linear and RBF kernels, AdaBoost, Random Forest, among others under the popular scikit-learn package. We also compare our methods with two bio-inspired methods; regarding evolutionary computation, we compare with EvoDAG a genetic programming system and PSMS a particle swarm optimization method. For instance, we found that our ensemble-based method KMSE achieves very competitive performances in almost all benchmarks, having the best mean rank among all compared methods under our set of benchmarks. Our single-instance KMS also performs competitively on average, yet using only a fraction of KMSE’s computational power.

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