

# AN ENHANCED CLASSIFICATION SYSTEM BASED ON KERNEL PRINCIPAL COMPONENT ANALYSIS AND DATA COMPLEXITY MEASURES

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**Abstract.** *Principal component analysis is commonly used as a pre-step before employing a classifier to avoid the negative effect of the dimensionality and multicollinearity. The performance of a classifier is severely affected by the deviations from the linearity of the data structure and noisy samples. In this paper, we propose a new classification system that overcomes the drawback of these crucial problems, simultaneously. Our proposal is relying on the kernel principal component analysis with a proper parameter selection approach with data complexity measures. According to the empirical results, F1, T2 and T3 in AUC, T3 in GMEAN and T2 and T3 in MCC performed better than classical and other complexity measures. Comparison of classifiers showed that Radial SVM performs better in AUC, and KNN performs better in GMEAN and MCC using KPCA with complexity measures. As a result, our proposed system produces better results in various classification algorithms with respect to classical approach.*

**Keywords:** *classification system; data complexity; kernel principal component analysis.*

## 1. INTRODUCTION

Classification systems have been used intensively to obtain the prediction of categorical responses for several areas such as bioinformatics [1-2], chemistry [3-4], medicine [5-7], ecology [8], and finance [9]. Due to the importance, the researchers aim to increase the accuracy of the classification results by improving the computational part of the classifiers.

During the classification process, it is an alternative way to employ PCA prior to the classifiers. The classifiers train the data using the compressed versions of the full features [10]. PCA is a preferable technique that extracts relevant components reflecting the variability of the full data [11]. It has attracted much attention to use PCA within the classification algorithms [12-17].

The classical PCA was designed to handle the linear projection on data [18]. In mostly cases, the data rely on a nonlinear structure. Classification systems are muchly sensitive to the structure of the data and it is necessary to use a method that can separate the data nonlinearly. Kernel PCA (KPCA) is a useful choice for such cases due to the nonlinear mapping capability [16,19]. KPCA was used to improve the classification performance of the models with several classifiers [20-23]. KPCA includes a kernel function and the proper selection of the parameters of this function should be carried out optimally [24-25]. However, the researchers

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ignored to select the optimal parameters of the kernel functions within KPCA related to the classifiers.

Aforementioned researches using KPCA do not take into account of data complexity to make dataset more separable. In this paper, we propose a novel approach to perform parameter selection in KPCA using the data complexity measures [26]. Our purpose is to select the kernel hyperparameters so as to achieve the maximal separation of the classes in the feature space. Hence, we aimed to tackle the dimensionality by separating classes harmonious with the distribution of the features. To the best of our knowledge, this study is the first attempt to present an objective way of the parameter selection in KPCA for the classification problems.

The paper is organized as follows: Section 2 gives a summary about theoretical background of KPCA. Section 3 introduces our proposed approach together with data complexities. Section 4 provides the experimental results that include the comparison of the traditional selection and our proposed way on several real data sets. Section 5 summarizes and discusses the obtained performance results.

## 2. KERNEL PRINCIPAL COMPONENT ANALYSIS

Let  $\phi(\mathbf{x})$  be a nonlinear transformation of  $\mathbf{x}$  with  $n$  data point and  $\mathbf{x}_i$  a  $d$ -dimensional vector. This transformation maps  $\mathbf{x}$  into a higher dimensional space ( $\mathbb{R}^m$ ,  $m > d$ ). Estimated standard principal components of  $\phi(\mathbf{x})$  are nonlinear principal components of  $\mathbf{x}$ . Assuming  $\sum_{i=1}^n \mathbf{x}_i = 0$  and  $\sum_{i=1}^n \phi(\mathbf{x}_i) = 0$ , we can write

$$S = \frac{1}{n} \sum_{i=1}^n \phi(\mathbf{x}_i) \phi(\mathbf{x}_i)^\top. \quad (1)$$

$S$  is the  $d \times d$  covariance matrix estimation of  $\phi(\mathbf{x})$ . Eigenvalues and eigen vectors of  $S$  satisfying

$$S\mathbf{V} = \lambda\mathbf{V}, \quad \lambda \geq 0 \quad (2)$$

need to be calculated. From Equation (1) and (2), we can write

$$\frac{1}{n} \sum_{i=1}^n \phi(\mathbf{x}_i) \{\phi(\mathbf{x}_i)^\top \mathbf{V}\} = \lambda \mathbf{V} \quad (3)$$

asnd

$$\mathbf{V} = \sum_i^n \alpha_i \phi(\mathbf{x}_i). \quad (4)$$

Substituting  $\mathbf{V}$  in Equation (3) with Equation (4), we have

$$\frac{1}{n} \sum_{i=1}^n \phi(\mathbf{x}_i) \left\{ \phi(\mathbf{x}_i)^\top \sum_i^n \alpha_i \phi(\mathbf{x}_i) \right\} = \lambda \sum_i^n \alpha_i \phi(\mathbf{x}_i). \quad (5)$$

We can define the function as

$$K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j). \quad (6)$$

Using Equation (5) and (6),

$$\frac{1}{n} \sum_{i=1}^n K(\mathbf{x}_i, \mathbf{x}_j) \sum_{j=1}^n \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) = \lambda \sum_{i=1}^n \alpha_i K(\mathbf{x}_i, \mathbf{x}_j) \quad (7)$$

$$K^2 \alpha = \lambda n K \alpha$$

$$K \alpha = \lambda n \alpha$$

Here  $\alpha$  is  $n$  dimensional column vector consisting of  $\alpha_i$ -s. Solving Equation (7) will allow us to calculate kernel principal components using

$$y(\mathbf{x}) = \phi(\mathbf{x})^\top \mathbf{V} = \sum_{i=1}^n \alpha_i K(\mathbf{x}, \mathbf{x}_i).$$

Kernel approach allows us to obtain principal components without calculating  $\phi(\mathbf{x})$ .

### 3. PARAMETER SELECTION BASED ON COMPLEXITY MEASURE

Kernels usually depend on a specific parameter. The selection of these parameters significantly affects the results. Therefore, correct parameter selection is important. We propose to use different complexity measures to determine the efficient kernel hyperparameter. The algorithm in Table 1 describes the approach for selecting optimal kernel hyperparameter. The aim of this approach is project dataset into higher dimensional space with lowest possible complexity.

**Table 1. Algorithm for obtaining KPCA radial kernel matrix with automated  $\sigma$  selection**

INPUT: $X_{train}, \sigma_{grid}, C$ (selected complexity measure)
1. For $\sigma$ in $\sigma_{grid}$ $X_{kpca}$ is calculated using $\sigma$ with radial kernel $C$ is calculated for $X_{kpca}$ and mapped into $C_{all}$
2. $\sigma_{opt}$ for optimum $C_{all}$ is determined.
OUTPUT: $X_{kpca}$ with $\sigma_{opt}$

#### 3.1. COMPLEXITY MEASURES

Lorena et al. [27] categorizes complexity into six category: overlapping, linearity, neighborhood, network, dimensionality, and class imbalance measures. KPCA is used to handle all these categories except class imbalance. Therefore, we used the first five category.

The overlapping measures examines the separation of classes. The problem is assumed to be simpler when at least one variable has discriminative values. Neighborhood measures

examines neighbors of data points and shape of decision boundary. Linearity measures the linear separability of the dataset. The problem is assumed to be simpler if it is linearly separable [28]. Network measures extracts structural information from the data set using graph methods [27]. Dimensionality measures are the measurement of data sparsity. They try to find if there are areas with low density, which is assumed to be hard to classify [29]. Table 2 gives the complexity measures used in the study.

Figure 1 shows an example of KPCA components constructed using different hyper parameter selection methods on banana dataset. Let us take an example of linear classifier. In banana dataset, it is almost impossible to discriminate classes using a linear classifier without KPCA. When we look at F2 kernel components, it is safe to tell that it is easier to model compared to no KPCA. Of course, we just see the first two dimensions. Linear separability is hard to see from high dimensions. The main point is that it is important to select the right complexity measure and it requires the researcher to have a good understanding of the dataset.

**Table 2. Complexity measure used in the study**

Category	Measure	Summary
Overlapping	Maximum Fisher's Discriminant Ratio (F1)	Largest discriminant ratio of all the variables.
	Volume of the overlapping region (F2)	The overlap of the distributions of the variables based on minimum and maximum values of variables for each class.
	Collective feature efficiency (F4)	A measurement of overlapping area of all variables.
Neighborhood	Fraction of borderline points (N1)	The percentage of vertexes incident to edges connecting examples of opposite classes in a Minimum Spanning Tree.
	Local Set Average Cardinality (LSC)	The set of points from the dataset whose distance of each example is smaller than the distance from the examples of the different class.
Linearity	Sum of the error distance by linear programming (L1)	The sum of the distances of incorrectly classified examples to a linear boundary used in linear SVM.
	Error rate of linear classifier (L2)	The error rate of the linear SVM classifier.
Network	Average Density of the network (Density)	The number of edges in the graph, divided by the maximum number of edges between pairs of data points.
	Clustering coefficient (ClsCoef)	The average clustering tendency of the vertexes by the ratio of existent edges between its neighbors and the total number of edges that could possibly exist between them.
	Hubs score (Hubs)	A measure of the influence of each node of the graph
Dimensionality	Average number of points per dimension (T2)	The ratio between the number of examples and dimensionality of the dataset.
	Average number of points per PCA (T3)	The ratio between the number of examples and the number of PCA components needed to represent 95 percent variability as the base of data sparsity assessment.
	Ratio of the PCA Dimension to the Original (T4)	The proportion of relevant and the original dimensions for a dataset.

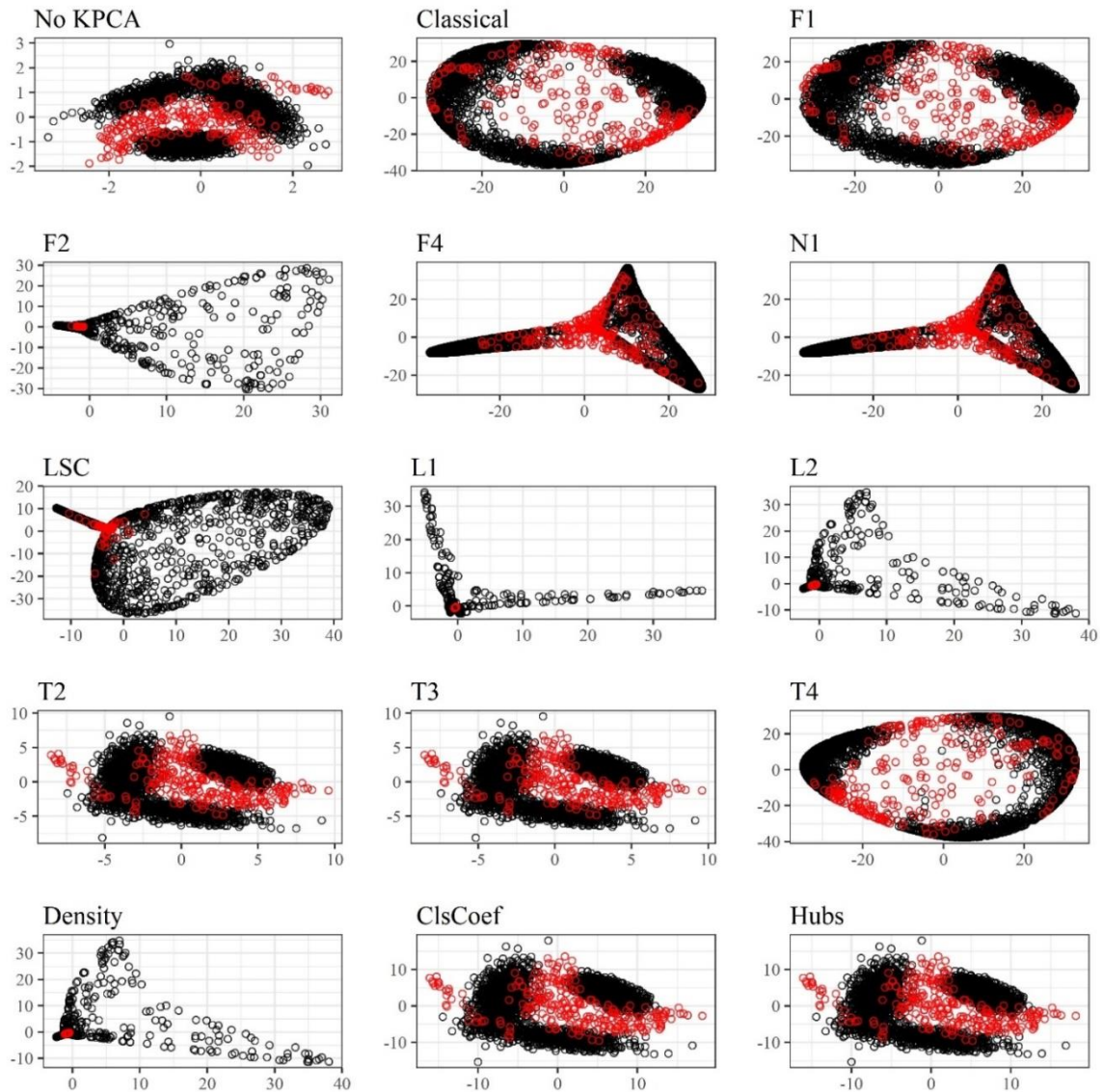


Figure 1. First two kernel principal components determined with different complexity measures for banana dataset.

#### 4. EXPERIMENTAL RESULTS

In this section we carried out extensive implementations on real data sets. On each experiment, we applied KPCA and obtained the principal component scores. Radial kernel function is used for KPCA and kernel hyperparameter is selected based on classical and proposed approaches. One of the parameter selection strategies in literature is chosen as classical approach [24]. In classical approach kernel hyperparameter is selected using

$$\sigma = 5 \cdot \text{mean}(d_i^{NN}).$$

Here,  $d_i^{NN}$  indicates distance from  $x_i$  to its nearest neighbor. Proposed approach used grid search where grid area is  $\{2^{-9}, \dots, 2^{10}\}$ . After obtaining the scores, we conducted 10 fold cross-validation for 10 times. The results were evaluated on test data with three well-known performance metrics: Area under the ROC curve (AUC), Matthews correlation coefficient

(MCC) and Geometric mean (G-Mean). All experiments were carried out using R software. The performance of our selection approach is examined using 13 benchmark data sets. The general properties of the data sets are given in Table 3. These datasets are easy to obtain from UCI and KEEL dataset repositories. Here,  $n$  is the number of samples,  $p$  is the number of features, and imbalance rate is  $\frac{n^{majority}}{n^{minority}}$ .

**Table 3. Datasets used in the study**

Datasets	$n$	$p$	Imbalance Rate
banana	2640	2	9.000
banknote	200	6	1.000
ecoli1	336	5	3.364
glass0	214	9	2.057
haberman	306	3	2.778
Ionosphere	351	32	1.786
iris0	150	4	2.000
kyphosis	81	3	3.765
newthyroid1	215	5	5.143
Vehicle1	846	18	2.881
Vehicle3	846	18	2.899
wisconsin	683	9	1.858
yeast4	1484	6	28.098

**Table 4. AUC values for different parameter selection strategies**

Datasets	Classifiers	Parameter Selection Strategy													
		classical	F1	F2	F4	N1	LSC	L1	L2	T2	T3	T4	Density	ClsCoef	Hubs
Banana	Naive Bayes	0.900	0.895	0.904	0.916	0.831	0.905	0.875	0.884	0.598	0.598	0.901	0.880	0.601	0.873
	Logistic regression	0.960	0.954	0.755	0.853	0.769	0.844	0.713	0.726	0.585	0.585	0.962	0.697	0.584	0.794
	CART	0.883	0.870	0.648	0.845	0.868	0.817	0.645	0.656	0.867	0.867	0.877	0.657	0.871	0.862
	J48	0.872	0.868	0.696	0.823	0.859	0.782	0.574	0.591	0.882	0.882	0.862	0.557	0.881	0.871
	Linear SVM	0.960	0.952	0.809	0.927	0.709	0.879	0.786	0.794	0.491	0.514	0.962	0.766	0.507	0.605
	Radial SVM	0.951	0.954	0.622	0.931	0.955	0.938	0.457	0.491	0.960	0.960	0.949	0.435	0.960	0.961
banknote	KNN	0.910	0.910	0.912	0.910	0.910	0.848	0.865	0.911	0.911	0.910	0.850	0.910	0.910	0.910
	Naive Bayes	0.932	0.994	0.567	0.994	0.992	0.994	0.988	0.988	0.994	0.994	0.992	0.563	0.566	0.602
	Logistic regression	0.003	0.002	0.004	0.002	0.002	0.002	0.004	0.004	0.002	0.002	0.002	0.004	0.004	0.009
	CART	0.786	0.942	0.553	0.942	0.942	0.942	0.946	0.946	0.942	0.942	0.969	0.548	0.550	0.562
	J48	0.794	0.954	0.542	0.953	0.953	0.954	0.955	0.955	0.954	0.954	0.956	0.539	0.539	0.550
	Linear SVM	0.003	0.999	0.014	0.999	0.999	0.999	0.997	0.997	0.999	0.999	0.997	0.004	0.004	0.009
ecoli1	Radial SVM	0.003	0.999	0.006	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.005	0.005	0.014
	KNN	0.995	0.995	0.988	0.995	0.994	0.995	0.993	0.993	0.995	0.995	0.992	0.990	0.989	0.959
	Naive Bayes	0.927	0.927	0.742	0.905	0.953	0.946	0.899	0.899	0.927	0.927	0.891	0.756	0.927	0.790
	Logistic regression	0.951	0.928	0.872	0.892	0.954	0.952	0.728	0.728	0.928	0.928	0.834	0.848	0.928	0.877
	CART	0.883	0.883	0.667	0.880	0.905	0.896	0.795	0.795	0.883	0.883	0.890	0.642	0.883	0.680
	J48	0.868	0.879	0.608	0.817	0.900	0.901	0.759	0.759	0.879	0.879	0.776	0.645	0.879	0.694
glass0	Linear SVM	0.941	0.927	0.128	0.932	0.949	0.949	0.574	0.569	0.927	0.927	0.931	0.419	0.927	0.479
	Radial SVM	0.924	0.896	0.129	0.922	0.940	0.945	0.873	0.873	0.896	0.896	0.916	0.407	0.896	0.476
	KNN	0.926	0.886	0.923	0.924	0.923	0.917	0.920	0.920	0.886	0.886	0.924	0.891	0.886	0.911
	Naive Bayes	0.677	0.809	0.512	0.793	0.662	0.699	0.712	0.712	0.809	0.809	0.791	0.531	0.732	0.801
	Logistic regression	0.731	0.844	0.800	0.684	0.758	0.732	0.717	0.717	0.844	0.844	0.692	0.691	0.714	0.841
	CART	0.732	0.806	0.512	0.815	0.722	0.748	0.747	0.747	0.806	0.806	0.816	0.538	0.771	0.808
haberman	J48	0.720	0.797	0.516	0.752	0.701	0.711	0.725	0.725	0.797	0.797	0.760	0.539	0.717	0.794
	Linear SVM	0.746	0.836	0.589	0.806	0.762	0.742	0.726	0.726	0.836	0.836	0.808	0.561	0.715	0.829
	Radial SVM	0.614	0.833	0.607	0.847	0.646	0.638	0.630	0.630	0.833	0.833	0.854	0.577	0.723	0.834
	KNN	0.811	0.854	0.749	0.853	0.788	0.808	0.804	0.804	0.854	0.854	0.853	0.659	0.843	0.855
	Naive Bayes	0.512	0.673	0.543	0.669	0.534	0.535	0.581	0.647	0.673	0.673	0.673	0.665	0.670	0.587
	Logistic regression	0.605	0.668	0.610	0.560	0.535	0.559	0.606	0.569	0.668	0.668	0.669	0.671	0.664	0.607
Ionosphere	CART	0.533	0.622	0.538	0.637	0.503	0.517	0.498	0.530	0.622	0.622	0.621	0.608	0.625	0.514
	J48	0.530	0.600	0.509	0.534	0.523	0.515	0.529	0.540	0.600	0.600	0.598	0.592	0.599	0.520
	Linear SVM	0.578	0.628	0.550	0.566	0.508	0.534	0.560	0.575	0.600	0.619	0.625	0.602	0.620	0.573
	Radial SVM	0.569	0.670	0.571	0.658	0.498	0.534	0.529	0.461	0.670	0.670	0.670	0.641	0.667	0.536
	KNN	0.505	0.630	0.585	0.629	0.510	0.515	0.579	0.632	0.630	0.630	0.630	0.628	0.628	0.624
	Naive Bayes	0.517	0.953	0.749	0.953	0.913	0.949	0.934	0.934	0.953	0.953	0.938	0.585	0.756	0.943
yeast4	Logistic regression	0.023	0.102	0.021	0.101	0.020	0.124	0.136	0.136	0.102	0.102	0.111	0.025	0.030	0.107
	CART	0.527	0.860	0.530	0.860	0.658	0.887	0.904	0.904	0.860	0.860	0.876	0.526	0.564	0.867
	J48	0.523	0.854	0.556	0.856	0.567	0.860	0.847	0.847	0.854	0.854	0.844	0.558	0.590	0.847
	Linear SVM	0.835	0.907	0.979	0.912	0.960	0.889	0.872	0.872	0.907	0.907	0.939	0.975	0.972	0.947
	Radial SVM	0.611	0.984	0.780	0.984	0.547	0.966	0.944	0.944	0.984	0.984	0.983	0.903	0.807	0.984



Datasets	Classifiers	Parameter Selection Strategy													
		Classical	F1	F2	F4	N1	LSC	L1	L2	T2	T3	T4	Density	ClsCoef	Hubs
J48	Naive Bayes	0.691	0.733	0.141	0.726	0.654	0.684	0.696	0.696	0.733	0.733	0.727	0.160	0.684	0.737
	Linear SVM	0.469	0.651	0.101	0.270	0.522	0.493	0.464	0.453	0.655	0.657	0.370	0.046	0.399	0.631
	Radial SVM	0.588	0.724	0.108	0.717	0.546	0.566	0.565	0.563	0.728	0.731	0.701	0.126	0.594	0.718
	KNN	0.723	0.755	0.591	0.746	0.675	0.702	0.699	0.699	0.755	0.755	0.741	0.318	0.740	0.754
haberman	Naive Bayes	0.188	0.522	0.379	0.586	0.263	0.270	0.435	0.541	0.522	0.522	0.522	0.530	0.515	0.519
	Logistic regression	0.121	0.476	0.121	0.461	0.121	0.141	0.202	0.445	0.476	0.476	0.476	0.450	0.467	0.252
	CART	0.154	0.472	0.264	0.487	0.100	0.162	0.245	0.383	0.472	0.472	0.472	0.432	0.468	0.254
	J48	0.113	0.523	0.221	0.489	0.121	0.122	0.251	0.426	0.523	0.523	0.522	0.498	0.518	0.276
Ionosphere	Naive Bayes	0.096	0.890	0.056	0.889	0.031	0.822	0.739	0.739	0.890	0.890	0.878	0.066	0.143	0.879
	Logistic regression	0.020	0.083	0.031	0.083	0.037	0.110	0.125	0.125	0.083	0.083	0.066	0.030	0.034	0.072
	CART	0.179	0.836	0.247	0.834	0.499	0.872	0.888	0.888	0.836	0.836	0.847	0.208	0.301	0.838
	J48	0.185	0.847	0.276	0.848	0.331	0.851	0.843	0.843	0.847	0.847	0.843	0.310	0.338	0.838
iris0	Naive Bayes	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.115	0.965	0.163
	Logistic regression	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.157	0.976	0.237
	CART	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.149	0.959	0.183
	J48	0.985	0.987	0.987	0.987	0.987	0.987	0.987	0.987	0.987	0.987	0.984	0.222	0.962	0.247
kyphosis	Naive Bayes	0.204	0.469	0.048	0.471	0.363	0.235	0.209	0.209	0.469	0.469	0.544	0.272	0.291	0.318
	Logistic regression	0.365	0.449	0.000	0.560	0.468	0.405	0.497	0.497	0.449	0.449	0.505	0.278	0.360	0.479
	CART	0.187	0.677	0.000	0.624	0.447	0.414	0.436	0.436	0.677	0.677	0.449	0.361	0.470	0.638
	J48	0.301	0.540	0.000	0.493	0.369	0.361	0.431	0.431	0.540	0.540	0.442	0.353	0.436	0.530
newthyroid1	Naive Bayes	0.010	0.820	0.268	0.819	0.822	0.895	0.828	0.828	0.820	0.820	0.824	0.234	0.150	0.193
	Logistic regression	0.000	0.913	0.235	0.912	0.913	0.931	0.900	0.900	0.913	0.913	0.911	0.213	0.016	0.042
	CART	0.009	0.805	0.215	0.804	0.805	0.788	0.823	0.823	0.805	0.805	0.814	0.197	0.061	0.138
	J48	0.012	0.911	0.300	0.912	0.905	0.838	0.919	0.919	0.911	0.911	0.911	0.260	0.103	0.194
Vehicle1	Naive Bayes	0.000	0.709	0.694	0.709	0.038	0.147	0.709	0.709	0.709	0.709	0.709	0.694	0.005	0.709
	Logistic regression	0.000	0.026	0.034	0.026	0.001	0.000	0.026	0.026	0.026	0.026	0.026	0.025	0.000	0.026
	CART	0.000	0.745	0.700	0.744	0.088	0.210	0.745	0.745	0.745	0.745	0.745	0.731	0.184	0.745
	J48	0.000	0.772	0.702	0.772	0.086	0.194	0.772	0.772	0.772	0.772	0.772	0.757	0.239	0.772
Vehicle3	Naive Bayes	0.000	0.672	0.505	0.672	0.657	0.672	0.672	0.672	0.672	0.672	0.672	0.011	0.011	0.005
	Logistic regression	0.000	0.272	0.134	0.272	0.266	0.272	0.272	0.272	0.272	0.272	0.272	0.000	0.000	0.000
	CART	0.000	0.489	0.324	0.489	0.477	0.489	0.489	0.489	0.489	0.489	0.489	0.038	0.037	0.017
	J48	0.000	0.512	0.288	0.512	0.500	0.512	0.512	0.512	0.512	0.512	0.512	0.068	0.063	0.050
wisconsin	Naive Bayes	0.109	0.948	0.329	0.947	0.775	0.954	0.949	0.949	0.948	0.948	0.948	0.949	0.148	0.109
	Logistic regression	0.780	0.936	0.958	0.932	0.958	0.907	0.912	0.912	0.936	0.936	0.936	0.913	0.921	0.838
	CART	0.089	0.974	0.109	0.974	0.614	0.964	0.964	0.964	0.974	0.974	0.974	0.965	0.187	0.089
	J48	0.109	0.955	0.135	0.954	0.638	0.947	0.950	0.950	0.955	0.955	0.955	0.950	0.142	0.109
yeast4	Naive Bayes	0.537	0.218	0.734	0.633	0.723	0.491	0.582	0.582	0.218	0.218	0.633	0.218	0.220	0.220
	Logistic regression	0.276	0.000	0.330	0.508	0.331	0.315	0.444	0.444	0.000	0.000	0.501	0.000	0.000	0.000
	CART	0.408	0.000	0.045	0.447	0.049	0.351	0.204	0.204	0.000	0.000	0.451	0.000	0.052	0.052
	J48	0.345	0.000	0.132	0.506	0.124	0.237	0.294	0.294	0.000	0.000	0.510	0.000	0.000	0.000
Banana	Naive Bayes	0.426	0.415	0.698	0.567	0.342	0.543	0.577	0.607	0.000	0.000	0.467	0.586	0.002	0.378
	Logistic regression	0.791	0.779	0.498	0.716	0.352	0.690	0.334	0.374	0.000	0.000	0.794	0.322	0.000	0.253
	CART	0.749	0.727	0.466	0.702	0.732	0.668	0.255	0.303	0.707	0.707	0.728	0.243	0.706	0.733
	J48	0.741	0.727	0.442	0.698	0.738	0.633	0.288	0.310	0.719	0.719	0.733	0.282	0.719	0.740
	Naive Bayes	0.791	0.773	0.018	0.709	0.124	0.508	0.001	0.008	0.000	0.000	0.798	0.001	0.002	0.142
	Linear SVM	0.800	0.796	0.434	0.777	0.779	0.761	0.320	0.346	0.758	0.758	0.796	0.328	0.759	0.770
	Radial SVM	0.269	0.000	0.339	0.177	0.350	0.309	0.128	0.126	0.000	0.000	0.206	0.000	0.000	0.009
	KNN	0.379	0.116	0.334	0.364	0.336	0.380	0.394	0.394	0.116	0.116	0.364	0.116	0.277	0.277

Table 6. MCC values for different parameter selection strategies

Datasets	Classifiers	Parameter Selection Strategy													
		Classical	F1	F2	F4	N1	LSC	L1	L2	T2	T3	T4	Density	ClsCoef	Hubs
Banana	Naive Bayes	0.426	0.415	0.698	0.567	0.342	0.543	0.577	0.607	0.000	0.000	0.467	0.586	0.002	0.378
	Logistic regression	0.791	0.779	0.498	0.716	0.352	0.690	0.334	0.374	0.000	0.000	0.794	0.322	0.000	0.253
	CART	0.749	0.727	0.466	0.702	0.732	0.668	0.255	0.303	0.707	0.707	0.728	0.243	0.706	0.733
	J48	0.741	0.727	0.442	0.698	0.738	0.633	0.288	0.310	0.719	0.719	0.733	0.282	0.719	0.740
	Naive Bayes	0.791	0.773	0.018	0.709	0.124	0.508	0.001	0.008	0.000	0.000	0.798	0.001	0.002	0.142
	Linear SVM	0.800	0.796	0.434	0.777	0.779	0.761	0.320	0.346	0.758	0.758	0.796	0.328	0.759	0.770
	Radial SVM	0.269	0.000	0.339	0.177	0.350	0.309	0.128	0.126	0.000	0.000	0.206	0.000	0.000	0.009
	KNN	0.379	0.116	0.334	0.364	0.336	0.380	0.394	0.394	0.116	0.116	0.364	0.116	0.277	0.277





Datasets	Classifiers	Parameter Selection Strategy													
		Classical	F1	F2	F4	N1	LSC	L1	L2	T2	T3	T4	Density	ClsCoef	Hubs
	CART	0.298	0.002	0.035	0.305	0.038	0.244	0.146	0.146	0.002	0.002	0.310	0.002	0.024	0.024
	J48	0.239	0.000	0.081	0.342	0.075	0.153	0.161	0.161	0.000	0.000	0.343	0.000	0.000	0.000
	Linear SVM	0.000	0.000	0.003	0.021	0.000	0.041	0.000	0.000	0.005	0.000	0.023	0.001	0.000	0.003
	Radial SVM	0.242	0.000	0.223	0.137	0.239	0.265	0.092	0.091	0.000	0.000	0.155	0.000	0.001	0.004
	KNN	0.268	0.072	0.219	0.257	0.221	0.256	0.277	0.277	0.072	0.072	0.258	0.072	0.171	0.171

The key point of the classification process is determined by the kernel hyperparameter selection approaches. We utilize 7 different classifiers and 13 different data complexity measures which shown in Table 3, 4, and 5. Table 3, 4, and 5 gives AUC, GMEAN and MCC values for each case. Different performance measures may find different approaches better. Some cases did not require any kernel hyperparameter selection as predictions were completely correct. However, there were cases which kernel hyperparameter selection is utmost importance. Datasets Haberman, ionosphere, and kyphosis are among these. Number of wins for parameter selection strategies in each classifier and each performance measure are counted and is given in Table 7. As an example, it should be read like this: F1 parameter selection strategy performed best 5 times using CART classifier in AUC for all datasets. These wins are based on Table 4, 5 and 6. Win count is increased 1 for each tie also. So total numbers can be more than 13, which is the number of datasets. In total wins, F1, T2, and T3 measures are performed better for AUC criteria. The same goes for T3 for GMEAN and T2 and T3 for MCC criteria. Table 8 gives total win numbers according to classifiers in a similar way to Table 7. Number of wins are the count of how many times a classifier performed best in each performance measure and each parameter selection strategy. An example of how to read numbers is: CART algorithm performed best 3 times using classical parameter selection strategy in AUC for all datasets. Total wins are total number of wins of all parameter selectino strategies. Based on total wins, Radial SVM performed better with all KPCA strategies in AUC. KNN performed better than other classifiers in GMEAN and MCC.

Radial SVM wins 56 times and is the best one in AUC performance. KNN performed better than other classifiers in GMEAN and MCC.

**Table 7. Number of wins for parameter selection strategies**

Performance measure	Classifier	Parameter selection strategy													
		Classical	F1	F2	F4	N1	LSC	L1	L2	T2	T3	T4	Density	ClsCoef	Hubs
AUC	CART	3	5	1	3	2	2	5	5	5	5	6	0	0	1
	J48	1	4	1	4	1	5	3	3	5	5	2	0	0	0
	KNN	3	3	3	2	3	1	2	3	3	3	4	1	0	2
	Linear SVM	1	7	2	5	2	4	3	3	6	6	5	0	0	1
	Logistic regresion	4	2	3	1	2	1	2	2	2	2	2	2	1	1
	Naive Bayes	1	8	1	5	2	3	3	3	8	8	6	0	1	2
	Radial SVM	0	5	1	3	2	3	2	2	5	5	3	0	0	1
	<b>Total</b>	<b>13</b>	<b>34</b>	<b>12</b>	<b>23</b>	<b>14</b>	<b>19</b>	<b>20</b>	<b>21</b>	<b>34</b>	<b>34</b>	<b>28</b>	<b>3</b>	<b>2</b>	<b>8</b>
GMEAN	CART	3	6	2	4	3	3	6	6	6	6	7	1	1	2
	J48	1	6	2	4	3	4	4	4	6	6	4	1	1	3
	KNN	3	6	4	4	3	4	4	4	6	6	5	1	1	2
	Linear SVM	4	3	2	3	2	4	1	1	2	3	1	0	0	0
	Logistic regresion	3	4	4	5	2	4	4	4	4	4	4	1	1	2
	Naive Bayes	2	5	2	3	1	4	4	4	5	5	4	1	0	1
	Radial SVM	1	1	1	3	3	2	2	2	1	3	1	0	0	1
	<b>Total</b>	<b>17</b>	<b>31</b>	<b>17</b>	<b>26</b>	<b>17</b>	<b>25</b>	<b>25</b>	<b>25</b>	<b>30</b>	<b>33</b>	<b>26</b>	<b>5</b>	<b>4</b>	<b>11</b>
MCC	CART	3	7	2	4	3	3	6	6	7	7	6	1	1	2
	J48	2	6	2	4	3	4	4	4	6	6	4	1	1	2
	KNN	3	5	3	4	3	3	3	3	5	5	4	2	1	2
	Linear SVM	3	3	1	3	1	4	2	1	3	3	2	0	0	1
	Logistic regresion	3	5	2	5	4	4	4	4	5	5	5	1	1	3
	Naive Bayes	1	4	3	2	1	5	3	4	4	4	4	0	0	0
	Radial SVM	1	1	1	4	2	3	1	2	2	2	2	0	0	0
	<b>Total</b>	<b>16</b>	<b>31</b>	<b>14</b>	<b>26</b>	<b>17</b>	<b>26</b>	<b>23</b>	<b>24</b>	<b>32</b>	<b>32</b>	<b>27</b>	<b>5</b>	<b>4</b>	<b>10</b>

**Table 8. Number of wins for classifiers**

Performance measure	Classifier	Parameter selection strategy													Total Wins	
		Classical	F1	F2	F4	N1	LSC	L1	L2	T2	T3	T4	Density	ClsCoef		Hubs
AUC	CART	3	1	1	1	1	1	1	1	1	1	1	0	0	0	13
	J48	2	0	0	0	0	0	0	0	0	0	0	0	0	0	2
	KNN	5	3	5	3	4	4	5	5	3	3	2	3	4	5	54
	Linear SVM	5	4	4	6	5	3	3	3	4	4	5	2	2	1	51
	Logistic regression	10	4	6	1	4	4	2	1	3	3	2	6	4	3	53
	Naive Bayes	3	4	2	2	2	2	3	4	4	4	3	2	2	1	38
	Radial SVM	2	6	1	7	3	5	4	4	6	6	7	1	1	3	<b>56</b>
GMEAN	CART	4	4	2	4	2	3	3	3	4	4	3	2	2	2	42
	J48	3	2	1	1	1	1	2	2	2	2	2	1	2	1	23
	KNN	8	4	7	5	6	5	3	3	5	5	5	7	8	8	<b>79</b>
	Linear SVM	4	3	2	2	2	2	2	2	3	3	2	2	1	1	31
	Logistic regression	6	2	3	2	5	3	4	4	2	2	3	1	2	2	41
	Naive Bayes	5	4	5	5	4	5	6	6	4	4	5	3	1	1	58
	Radial SVM	3	2	0	1	1	2	0	0	1	1	1	0	0	1	13
MCC	CART	4	3	1	3	1	2	2	2	3	3	2	1	1	1	29
	J48	2	1	0	1	0	0	0	0	1	1	2	0	1	0	9
	KNN	8	3	7	4	4	4	6	6	4	4	4	6	7	7	<b>74</b>
	Linear SVM	4	3	2	3	2	2	3	3	3	3	3	1	0	2	34
	Logistic regression	5	2	3	2	6	3	3	3	2	2	2	1	2	1	37
	Naive Bayes	4	2	2	2	2	3	3	3	2	2	3	3	0	0	31
	Radial SVM	3	3	2	2	2	3	0	0	2	2	1	1	2	2	25

## 5. CONCLUSION

KPCA is a form of PCA which can identify nonlinear structure of dataset. The kernel hyperparameters in KPCA play a major role in the emergence of this structure. Therefore, it is important to choose these parameters correctly. We suggested that these parameters can be estimated accurately using measures of complexity. We summarized the results we obtained from 7 different classifiers and 13 different data sets in Table 7. Measures F1, T2 and T3 were found to be more successful than other measures. Also, classical parameter selection clearly performed worse than all complexity measure approaches. Therefore, we recommend this approach to researchers who will use KPCA.

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