SUPPORT VECTOR MACHINES FOR CLASSIFICATION OF SOILS ACCORDING TO GEOGRAPHIC ORIGIN BASED ON THEIR RADIONUCLIDE CONTENT

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Abstract: The paper introduces support vector machines (SVM), a recent method in statistical learning theory, used to recognize and classify soils according to their geographic origin. The classification was performed based on activities of seven radionuclides determined by gamma-ray spectrometry. The radionuclides of uranium and thorium series (^{226}Ra, ^{232}Th, ^{235}U, ^{238}U) and ^{40}K were used to differentiate investigated areas based on geology, while cosmogenic beryllium (^{7}Be) and anthropogenic ^{137}Cs were used to differentiate areas according to their susceptibility to fallout. The performances of the proposed method was compared to those of principal component analysis (PCA), linear discriminant analysis (LDA), k-nearest neighbours (kNN), soft independent modelling of class analogy (SIMCA) and artificial neural networks (ANN) applied to the same dataset.

Key words: Chemometrics; Lithology; Fallout; Prediction ability

1. Introduction

There are a number of well known and widely used methods for analysis of spatially dependent data. Chemometric analysis methods provide powerful tools for the analysis of environmental data which are characterized by strong variation of the element concentration in environmental compartments due to natural inhomogenities and complexity of interactions

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within variables (Einax et al., 1997; Dragović et al., 2007). There are only few studies on employing the chemometric approach in spatial data analysis of radioactively contaminated areas (Kanevski et al., 1996, 1997; Kanevski, 2008; Kanevski et al., 2009).

Support vector machines (SVM) belong to new generation of learning algorithms used for classification and regression tasks (Vapnik, 1995, 1998; Xu et al., 2006). They have been introduced in chemometrics firstly to resolve mid and near infrared classification tasks (Belousov et al., 2002; Devos et al., 2009).

In addition to different classification applications of SVM in a wide variety of environmental sciences, there are a lot of researches based on SVM which are dealing with optimal sample selection in classification (Zomer et al., 2004). For the purpose of estimation of the performance of SVM, many authors have judged this learning theory against artificial neural networks (ANN), very often obtaining opposite results (King et al., 2000, Li et al., 2006). In available literature there are no data on application of SVMs in classification of soils in respect to their radioactivity.

The objective of this study was to test the efficiency of SVM in discrimination of soil samples from Serbia and Montenegro according to geographic origin. Soil samples were analyzed by gamma-ray spectrometry and then classified according to their origin based on their radionuclide content. The specific levels of natural environmental radiation are related to the geological composition of each lithologically separated area, and to the content of natural radionuclides in rocks the soils originate from (UNSCEAR, 2000). Geologically, the territory of Serbia and Montenegro includes a great number of rock complexes (magmatic, sedimentary and metamorphic rocks) which are markedly different in respect to their age, genesis, mineral content and petrochemical and geochemical characteristics. Outstanding differences in natural radioactivity of soils can be connected with their geological origin (Dimitrijević, 1995). Therefore, the set of natural radionuclides (226Ra, 238U, 235U, 40K and 232Th) was used in this work to differentiate investigated areas based on geology. In addition to natural radionuclides in all soil samples a man-made radionuclide, 137Cs, derived from Chernobyl accident was also determined, which activity could be influenced by altitudes of sampling areas. Ecosystems at high alitudes are predisposed to receive higher fallout because of high precipitation rates which enhance the likelihood of deposition (Howard et al., 1991). In analyzed soil samples the cosmogenic radionuclide 7Be was also detected. The activities of this radionuclide on the ground are higher in areas of high rainfall. Since the precipitation level is generally higher in upland regions, an increase in concentration of beryllium with altitude is to be expected (Salisbury and Cartwright, 2005). Therefore, radiocesium and beryllium were used in our work to differentiate areas according to their susceptibility to fallout.

2. Materials and methods

2.1. Samples

A total of 103 samples including six to eight subsamples of surface soils were collected from fifteen geographic regions of Serbia and Montenegro in 2003. The geographic coordinates of sampling locations and the distribution of samples per location is shown in Table 1. After removal of vegetation and other debris samples were dried to constant weight and passed through a 2 mm mesh sieve. Prior to gamma-ray spectrometry measurements, the homogenized samples were stored in 1L Marinelli beakers for one month to ensure equilibrium between ^{226}Ra and its daughters.

Table 1. Geographic coordinates of locations and number of samples per each location

Sampling location no.	Location	Geographic coordinates (Northing, Easting)	Number of samples
1	Slatina	N 42° 45’, E 19° 46’	7
2	Beljanica	N 44° 06’, E 21° 42’	6
3	Željevica	N 42° 46’, E 19° 46’	6
4	Kopaonik	N 43° 17’, E 20° 48’	10
5	Avala	N 44° 41’, E 20° 31’	6
6	Devojački Bunar	N 45° 00’, E 20° 57’	8
7	Bukulja	N 44° 18’, E 20° 31’	8
8	Kosmaj	N 44° 28’, E20° 33’	7
9	Stara Planina	N 43° 24’, E 22° 39’	5
10	Surdulica	N 42° 41’, E 22° 10’	5
11	Bogićevica	N 42° 36’, E 20° 04’	6
12	Durmitor	N 43° 09’, E 19° 07’	8
13	Kosovska Kamenica	N 42° 35’, E 21° 34’	7
14	Kukavica	N 42° 47’, E 21° 56’	5
15	Loznica	N 44° 32’, E 19° 14’	9

2.2. Radioactivity measurements

Measurements were performed using an HPGe gamma-ray spectrometer ORTEC-AMETEK (model GEM 25) of 34% relative efficiency and 1.65 keV FWHM for ^{60}Co at 1.33 MeV. All samples were measured for 60 ks. The spectra obtained were processed using Gamma Vision 32 software (ORTEC, 2001).

The ^{238}U activity was evaluated through gamma ray emission at 63.3 keV (branching 4.8%) of its daughter ^{234}Th, neglecting the 63.8 keV gamma ray from ^{232}Th, which has a branching as low as 0.27%. For the determination of ^{235}U activity the gamma ray line at 143.8 keV was used. The ^{226}Ra activity was determined through the gamma ray energies at 295.2 and 351.9 keV of ^{214}Pb and those at 609.3, 1120.3 and 1764.5 keV of ^{214}Bi. For the measurements of the ^{232}Th activity, the gamma ray lines at 911.1 and 969.1 keV of ^{228}Ac were used. The ^{137}Cs, ^{40}K and ^{7}Be isotopes were directly measured at 661.7, 1460.8 and 477.6 keV, respectively. Background spectral intensities were determined before sample measurements and substracted from corresponding sample intensities. For quality assurance purposes checks on calibration were performed using standard reference materials and proficiency test on the determination of gamma emitting radionuclides (IAEA, 2007).

2.3. Support vector machines

A SVM represents state-of-the-art learning approach to pattern classification and it is based on *binary classification model* (Vapnik, 1995). Binary model assumes that a soil sample belongs to just one class and that there are only two classes ($C = \{c_1, c_2\}$). Usually c_1 and c_2 are called positive and negative classes respectively. Each classification task with n classes can be modelled as a sequence of $\binom{n}{2}$ binary tasks using the *one-versus-one* approach in which one trains $n*(n-1)/2$ binary classifiers, one for each pair of classes. The final decision is made using voting i.e. a class that is predicted the most is selected as an output. Let $(\mathbf{x}_i, y_i),\ \mathbf{x}_i \in R^n,\ y_i \in \{-1,1\},\quad i = 1,...,m$ be the training set. Fig. 1 is used to explain the basic idea of the SVM classification. White and grey squares represent samples from a training set comprised of two distinct classes.

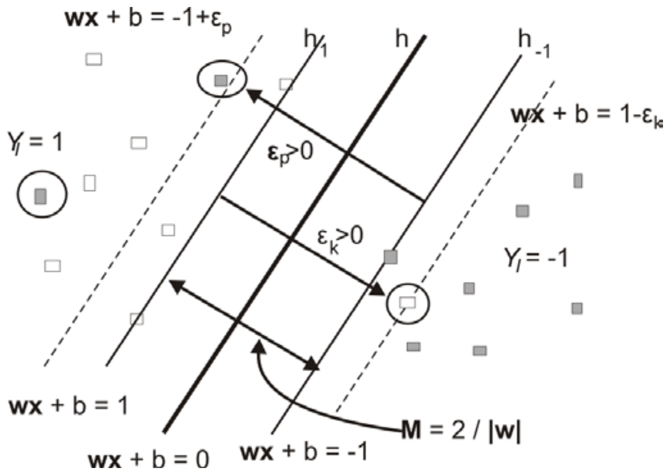

Fig. 1. SVM used for classification: construction of a separation hyper-plane in a two dimensional case (hyper-plane is here a line).

For a moment assume that classes are linearly separable, i.e. neglect circled examples in Fig. 1. During the learning phase one seeks a separating hyper-plane which best separates the examples of two classes. Let h_1: $\mathbf{w} \cdot \mathbf{x} + b = 1$ (where "." denotes the dot product) and h_{-1}: $\mathbf{w} \cdot \mathbf{x} + b = -1$, $\mathbf{w}, \mathbf{x} \in R^n, b \in R$, are possible hyper-planes so that all white examples lie above h_1 ($y_i = 1$) and all grey examples lie under h_{-1}. ($y_i = -1$). Hence for all training examples ($\mathbf{x}_i$, y_i) it follows that:

$$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1, \quad i = 1,2,...m \tag{1}$$

One chooses h: $\mathbf{w} \cdot \mathbf{x} + b = 0$ to be the best separating hyper-plane lying in the middle between already-fixed hyper-planes h_1 and h_{-1}. The notion of the best separation can be formulated to find the maximum margin M that separates data from both classes. Since the margin is equal to $\frac{2}{\|\mathbf{w}\|}$, maximizing the margin is equal to minimizing $\|\mathbf{w}\|$. The best separating hyper-plane can now be found by solving the following nonlinear convex programming problem (for solving optimization problem see Fletcher, 1987): find **w**, *b* to be

$$\begin{aligned} &\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2 \\ &\text{w.r.t}: 1\text{-}\, y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \leq 0, \quad i = 1,2,...m \end{aligned} \tag{2}$$

In practical classification problems, examples are usually not linearly separable (circled examples from Fig. 2). Therefore, the additional positive slack variables ε_i are introduced, which represent the distances of points on the wrong side of the separating hyper-plane (circled squares). The nonlinear convex program (2) now becomes:

$$\begin{aligned}&\min_{\mathbf{w},b}\ \frac{1}{2}\|\mathbf{w}\|^2+C\sum_i \varepsilon_i\\&\text{w.r.t}: 1-\varepsilon_i-y_i(\mathbf{w}\cdot\mathbf{x}_i+b)\le 0,\\&-\varepsilon_i\le 0,\quad i=1,2,...m\end{aligned} \tag{3}$$

Parameter C models the penalty for misclassified points in a training set. One wants to find a hyper-plane to minimize misclassification errors while maximizing the margin between the classes. The optimization problem (3) is usually solved in its dual form and the solution is:

$$\mathbf{w}^*=\sum_{i=1}^{m}\alpha_i y_i \mathbf{x}_i\ ,\ C\ge\alpha_i\ge 0,\quad i=1,...m \tag{4}$$

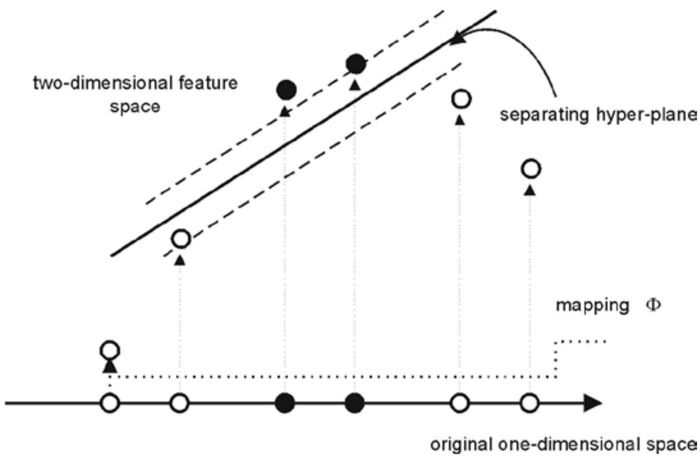

Fig. 2. Mapping examples (here one-dimensional) into high dimensional space (here two-dimensional).

Here a solution $\mathbf{w}^*$ for an optimal hyper-plane is a linear combination of training examples. However, it can be shown that $\mathbf{w}^*$ represents a linear combination of those vectors $\mathbf{x}_i$ (*support vectors*) for which the corresponding α_i are non-zero values. Support vectors for which $C>\alpha_i>0$ holds belong either to h_1 or h_{-1} (depending on y_i). Let $\mathbf{x}_a$ and $\mathbf{x}_b$ be two support vectors ($C>\alpha_a,\alpha_b>0$) for which holds $y_a = 1$ and $y_b = -1$. Now $b^*=-\frac{1}{2}\mathbf{w}^*\cdot(\mathbf{x}_a+\mathbf{x}_b)$ and finally classification function becomes:

$$f(\mathbf{x})=\operatorname{sgn}\sum_{i=1}^{m}\alpha_i y_i(\mathbf{x}_i\cdot\mathbf{x})+b^* \tag{5}$$

In order to cope with nonlinearity of the classification problem, SVM approach goes one step further. One can define the mapping of examples in a so-called *feature space* of very high dimension: $\phi : R^n \to R^d$, $n << d$ i.e. $\mathbf{x} \to \phi(\mathbf{x})$. The basic idea of this mapping into high dimensional space is to transform the non-linear case into linear one as illustrated in Fig. 2 and then to use already explained linear algorithm. In such a space dot-product from (5) transforms into $\phi(\mathbf{x}_i) \cdot \phi(\mathbf{x})$. It is known that there is a certain class of functions called *kernels* (Burges 1998) for which $k(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x}) \cdot \phi(\mathbf{y})$, which means that they represent dot-products in some high dimensional spaces, but can be easily computed in the input space. Using kernels (5) becomes:

$$f(\mathbf{x}) = \operatorname{sgn} \sum_{i=1}^{m} \alpha_i y_i k(\mathbf{x}_i, \mathbf{x}) + b^* \tag{6}$$

In all SVM experiments presented in this paper, an open-source package LIBSVM (Chang and Lin, 2001) as a standard implementation for SVM classification and regression algorithms was used. A detailed review of SVM for pattern classification can be found in Burges (1998).

3. Results and discussion

The basic statistics of activities of ^{226}Ra, ^{238}U, ^{235}U, ^{40}K, ^{137}Cs, ^{232}Th and ^{7}Be in analyzed soil samples by sampling locations is presented in Table 2. The range of natural radionuclide concentrations is a consequence of the variety of lithological components in the investigated areas. The highest activities of radionuclides of uranium and thorium series were measured in soil samples belonging to sedimentary formations as well as in soil samples that stem from magmatic rock complexes of silica oversaturated category. Numerous surveys worldwide have shown that the presence of radioactive elements in soils is strongly conditioned by those existing in the parent material, although the percentage of an element can vary in a given rock as a function of the process to which it has been subjected. The influence on the parent material and physicochemical phenomena associated with its weathering on concentrations of natural radionuclides in soil has been demonstrated in survey conducted by Baeza et al. (1995). Activity concentrations of natural radionuclides in Mediterranean soils have found to be lithologically-dependent (Schoorl et al., 2004; Laubenstein and Magaldi, 2008). Navas et al. (2005) have also shown that natural radioactivity of soils is largely controlled by the mineral composition of the parent material.

Table 2. Basic statistics of radionuclide activity concentrations (Bq kg-1 d.w.) in soils from different sampling locations

Radio-nuclide	Para-meter	Sampling location														
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
^{226}Ra	Mean	17.8	37.8	25.5	25.0	29.8	18.3	38.2	34.0	32.1	37.4	49.2	44.7	23.3	31.6	25.6
	SD	1.55	2.68	1.76	1.16	1.95	2.37	2.43	1.80	1.17	1.47	4.00	2.09	1.31	1.45	1.60
	Min	15.9	34.5	23.4	23.2	27.6	13.6	35.2	31.8	30.8	35.8	45.1	41.5	21.4	29.3	23.3
	Max	19.8	41.9	27.5	26.5	32.7	20.9	41.6	36.9	33.8	38.7	54.9	47.2	24.9	32.7	28.0
^{235}U	Mean	0.72	1.49	0.63	1.16	1.45	0.90	1.63	1.47	1.47	1.72	2.45	2.00	1.09	1.41	1.18
	SD	0.04	0.19	0.11	2.10	0.07	0.09	0.14	0.05	0.04	0.07	0.14	0.11	0.05	0.05	0.03
	Min	0.67	1.25	0.51	1.07	1.34	0.80	1.37	1.38	1.42	1.64	2.20	1.84	1.00	1.35	1.14
	Max	0.78	1.82	0.81	1.24	1.54	1.04	1.78	1.54	1.54	1.78	2.61	2.15	1.14	1.49	1.26
^{238}U	Mean	16.0	32.8	25.0	22.7	31.1	16.7	37.6	33.3	31.5	37.6	49.8	43.1	21.9	30.7	25.2
	SD	1.15	3.01	1.69	0.06	0.66	0.98	2.62	1.57	1.54	1.10	3.84	2.60	0.92	0.77	1.48
	Min	14.6	30.3	23.2	19.9	30.2	15.6	34.3	30.2	30.0	36.1	43.5	39.5	20.5	29.5	23.4
	Max	17.7	38.4	27.7	27.7	31.8	18.8	41.9	35.3	33.5	38.9	53.4	46.1	23.1	31.4	27.3
^{232}Th	Mean	23.5	47.5	32.1	35.9	40.6	21.3	44.6	43.9	36.0	47.5	47.6	77.0	32.6	44.7	37.5
	SD	1.18	4.84	4.80	2.85	2.03	2.03	2.43	1.56	1.64	1.84	1.70	4.24	2.09	2.30	1.67
	Min	22.4	40.3	26.3	30.5	37.1	18.3	41.5	41.4	33.6	45.6	45.3	71.0	30.2	41.1	35.2
	Max	25.0	53.6	37.7	40.1	42.5	24.5	48.9	45.9	38.1	50.6	49.5	83.4	35.5	46.8	40.3
^{40}K	Mean	422	520	345	580	686	332	652	710	645	651	882	298	655	755	548
	SD	17.4	43.2	22.8	22.0	25.7	21.6	57.6	16.8	29.7	19.2	25.8	21.4	19.8	31.0	24.6
	Min	392	468	314	550	645	301	537	686	610	629	847	271	633	723	500
	Max	442	578	366	611	710	360	705	728	672	679	919	328	677	791	593
^{137}Cs	Mean	30.5	15.7	84.7	25.8	77.8	60.0	101	41.3	5.60	40.3	42.8	61.8	60.2	13.8	43.2
	SD	2.00	2.03	3.87	1.86	1.61	4.82	8.53	1.31	0.29	1.38	2.53	2.96	3.16	0.22	3.07
	Min	27.5	13.2	80.9	23.5	75.1	52.7	89.7	39.8	5.25	38.4	40.6	58.4	55.9	13.5	38.1
	Max	32.8	18.9	91.8	29.5	79.9	64.5	112	43.2	5.88	41.8	46.8	68.4	65.0	14.0	46.8
^{7}Be	Mean	2.58	1.69	1.48	1.55	1.09	0.82	2.43	3.68	0.77	0.80	3.06	3.57	0.67	1.44	0.72
	SD	0.37	0.08	0.13	0.17	0.09	0.13	0.17	0.30	0.09	0.06	0.18	0.08	0.09	0.06	0.09
	Min	2.09	1.58	1.32	1.26	0.93	0.56	2.14	3.11	0.67	0.73	2.82	3.46	0.54	1.38	0.61
	Max	3.02	1.78	1.65	1.78	1.20	0.98	2.66	3.94	0.89	0.88	3.29	3.70	0.79	1.50	0.86

The variety of activity concentrations of ^{137}Cs and ^{7}Be was also observed in investigated soils depending on altitudes of sampling sites. A significant correlation between the accumulated deposition of man-made radionuclides (^{137}Cs, ^{238}Pu, $^{239+240}$Pu and ^{241}Am) in soils and altitudes of sampling sites has been reported in studies conducted worldwide (Bunzl and Kracke, 1988; Blagoeva and Zikovsky, 1995; Legarda et al., 2001; Arapis and Karandinos, 2004). However, factors other than altitude, such as physical, chemical and biological properties of soil, influence the behaviour of any radionuclide in the soil, as well as its migration velocity.

Shapiro-Wilk's test (significance level α was 0.05) (Shapiro and Wilk, 1965) for normality of activity distribution within each radionuclide was applied prior to any classification and revealed normal distribution of the data.

For classification purposes Gaussian kernel $k(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{2\sigma^2}\right)$ and linear kernel (no mapping, equation (5)) were used. After removing all training data that are not support vector points and retraining the classifier, the same solution will be obtained. Hence, support vectors represented the examples from the training set that best describe the classes. The ability to distinguish between support vectors and noisy data points enabled SVM to increase its generalization capacity in the learning process.

To test the quality of proposed classification method the *linear accuracy* measure defined as ratio of the number of correctly classified samples to the number of samples in test set was used.

In order to assure numerical stability of SVM classification, algorithm values of all parameters in data set were transformed to be roughly between -2 and 2 by applying the log transformation. A SVM classifier with Gaussian kernel was compared to a classifier with the linear kernel. Kernel parameter *gamma* and penalty *C* were varied from the following values {0.1, 0.5, 1, 2} and {1, 10, 20, 50, 100, 1000} respectively.

Results obtained after applying SVM to radionuclide data set are presented in Table 3. From this table it is evident that the performance of the Gaussian kernel is nearly identical to the linear one. This was a very interesting finding which indicates that the soil data points were linearly separable in the space of seven properties presented by seven radionuclides determined in soil samples. Therefore it was decided to use only linear kernel classifier in the remaining train-test splits (only parameter C needed). One can see that the linear SVM perfectly classifies our soil samples into 15 predefined classes – geographical areas.

Table 3. SVM classification performance: in the first two splits both Gaussian and linear kernel SVM were tested

Train-Test split	Gamma	C	Gaussian accuracy (%)	C	Linear accur. (%)
25 – 78	1	10	94.87	100	93.56
35 – 68	0.5	100	97.06	50	97.06
45 – 58				20	98.28
55 – 48				10	100
65 – 38				10	100
75 – 28				10	100
85 – 18				10	100

In Fig. 3 a comparison of prediction abilities of SVM and other pattern recognition methods applied to the same data set is presented. By applying PCA to experimental data, the classification rate of 86% was achieved (Dragović and Onjia, 2006). The application of linear discriminant analysis (LDA) as linear and parametric method, which maximizes the variance between classes and minimizes the variance within the classes, resulted in 82.8% of correctly classified samples (Dragović and Onjia, 2007). When a non-parametric method, k-nearest neighbours (kNN), was applied the classification rate of 88.6% was obtained. The results obtained by soft independent modelling of class analogy (SIMCA) method were very poor compared to those of other methods, giving only 60.0% of correct assignation for samples from test set. A back-propagation ANN classifier, designed by an input layer consisting of the radionuclide activities in the soil samples, a hidden layer and an output layer, composed of regions the samples were collected from, resulted in a classification rate of 92.1%. The prediction ability obtained with SVM was 93.6 to 100% depending on the number of samples in the test set.

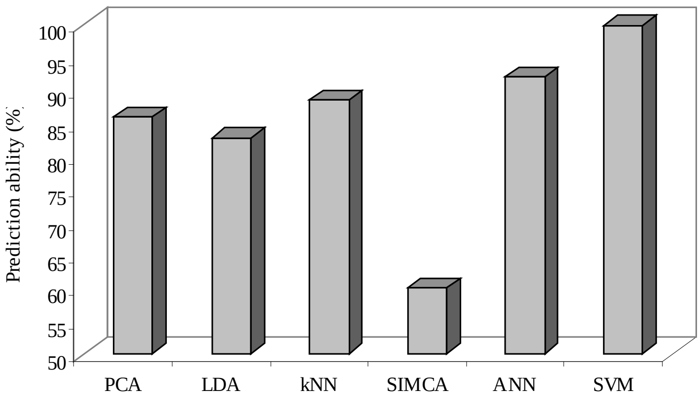

Fig. 3. Prediction ability of SVM in comparison to other pattern recognition methods applied to the same data set

The advantage of the SVM method over the ANN one became obvious in our problem setting: while in the ANN model one must choose between different topologies, a set of initial weights, learning rate, momentum and possibly other parameters, in the SVM approach one needs only one parameter (or two in the case of Gaussian kernel), and yet SVM will always find a global minimum (of error function) if it exists. In the case of ANN, initial random weights usually lead us to local optima.

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