LETTER **Communicated by Klaus Brinker**

Neighborhood Property–Based Pattern Selection for Support Vector Machines

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The support vector machine (SVM) has been spotlighted in the machine learning community because of its theoretical soundness and practical performance. When applied to a large data set, however, it requires a large memory and a long time for training. To cope with the practical difficulty, we propose a pattern selection algorithm based on neighborhood properties. The idea is to select only the patterns that are likely to be located near the decision boundary. Those patterns are expected to be more informative than the randomly selected patterns. The experimental results provide promising evidence that it is possible to successfully employ the proposed algorithm ahead of SVM training.

1 Introduction

The support vector machine (SVM) has been spotlighted in the machine learning community because of its theoretical soundness and practical performance. SVM has been highly successful in practical applications as diverse as face detection and recognition, handwritten character and digit recognition, text detection and categorization (Byun & Lee, 2002; Dumais, 1998; Heisele, Poggio, & Pontil, 2000; Joachims, 2002; Moghaddam & Yang, 2000; Osuna, Freund, & Girosi, 1997; Schölkopf, Burges, & Smola, 1999). However, when applied to a large data set, SVM training can become computationally intractable. In the formulation of SVM quadratic programming (QP), the dimension of the kernel matrix ($M \times M$) is equal to the number of training patterns (M) (Vapnik, 1999). Thus, when the data set is huge, training cannot be finished in a reasonable time, even if the kernel matrix could be loaded on the memory. Most standard SVM QP solvers have a time complexity of $O(M^3)$: MINOS, CPLEX, LOQO, and MATLAB QP routines. And the solvers using decomposition methods have a time complexity of

$I \cdot O(Mq + q^3)$, where I is the number of iterations and q is the size of the working set: Chunking, SMO, SVM^{light}, and SOR (Hearst, Schölkopf, Dumais, Osuna, & Platt, 1997; Joachims, 2002; Schölkopf et al., 1999; Platt, 1999). Needless to say, I increases as M increases. Empirical studies have estimated the run time of common decomposition methods to be proportional to $O(M^p)$, where p varies from approximately 1.7 to 3.0 depending on the problem (Hush, Kelly, Scovel, & Steinwart, 2006; Laskov, 2002). Moreover, SVM requires heavy or repetitive computation to find a satisfactory model: for instance, which kernel is favorable over the others (among RBF, polynomial, sigmoid, and others) and, additionally, how to choose the kernel parameters (width of basis function, polynomial degree, offset, and scale, respectively). There has been a considerable amount of work related to this topic, referred to as kernel learning, hyperkernels, and kernel alignment, for example (see Ong, Smola, & Williamson, 2005, and Sonnenburg, Rätsch, Schäfer, & Schölkopf, 2006). But the most common approaches for parameter selection are dependent on (cross–) validation. This implies one should train an SVM model multiple times until a proper model is found.

One way to circumvent this computational burden might be to select some training patterns in advance. One of the distinguishable merits of SVM theory is that it clarifies which patterns are important to training. These patterns are distributed near the decision boundary, and fully and succinctly define the classification task at hand (Cauwenberghs & Poggio, 2001; Pontil & Verri, 1998; Vapnik, 1999). Furthermore, the subset of support vectors (SVs) is almost identical regardless of which kernel function is chosen for training (Schölkopf, Burges, & Vapnik, 1995). From a computational point of view, it is therefore worth identifying a subset of would-be SVs in preprocessing, and then training the SVM model with the smaller set.

There have been several approaches to pattern selection that reduce the number of training patterns. Lyhyaoui et al. (1999) proposed the 1-nearest neighbor, searching from the opposite class after class-wise clustering. But this method presumes no possible class overlap in the training set to find the patterns near the decision boundary. Almeida, Braga, and Braga (2000) conducted k-means clustering. A cluster is defined as homogeneous if it consists of the patterns from the same class and heterogeneous otherwise. All of the patterns from a homogeneous cluster are replaced by a single centroid pattern, while the patterns from a heterogeneous cluster are all selected. The drawback is that it is not clear how to determine the number of clusters. Koggalage and Halgamuge (2004) also employed clustering to select the patterns from the training set. Their approach is quite similar to Almeida et al.'s (2000): clustering is conducted on the entire training set first, and the patterns are chosen that belong to the heterogeneous clusters. For a homogeneous cluster, on the contrary, the patterns along the rim of cluster are selected instead of the centroid of Almeida et al. (2000). It is a relatively safer approach since even in homogeneous clusters, the patterns near the decision boundary can exist if the cluster's boundary is almost in contact

with the decision boundary. But, it has a relative shortcoming as well, in that the patterns far away from the decision boundary are also picked as long as they lie along the rim. Furthermore, the setting of the radius and defining of the width of the rim are still unclear. In the meantime, for the reduced SVM (RSVM) of Lee and Mangasarian (2001), Zheng, Lu, Zheng, and Xu (2003) proposed using the centroids of clusters instead of random samples. It is more reasonable since the centroids are more representative than random samples. However, these clustering-based algorithms have a common weakness: the selected patterns are fully dependent on clustering performance, which could be unstable. Liu and Nakagawa (2001) made a related performance comparison. Sohn and Dagli (2001) suggested a slightly different approach. It utilizes fuzzy class membership through k nearest neighbors. The score of fuzzy class membership is translated as a probability of how deeply a pattern belongs to a class. By the scores, the patterns having a weak probability are eliminated from the training set. However, it overlooks the importance of the patterns near the decision boundary; they are equally treated to outliers (noisy pattern far from the decision boundary).

Active learning shares this issue of significant pattern identification with pattern selection (Brinker, 2003; Campbell, Cristianini, & Smola, 2000; Schohn & Cohn, 2000). However, there are substantial differences between them. First, the primary motivation of active learning comes from the high cost of obtaining labeled training patterns, not from that of training itself. For instance, in industrial process modeling, obtaining even a single training pattern may require several days. In e-mail filtering, obtaining training patterns is not expensive, but it takes many hours to label them. In pattern selection, however, the labeled training patterns are assumed to already exist. Second, active learning alternates between training with a newly introduced pattern and making queries over the next pattern. On the contrary, pattern selection runs only once before training as a preprocessor.

In this letter, we propose the neighborhood property—based pattern selection algorithm (NPPS). The practical time complexity of NPPS is vM, where v is the number of patterns in the overlap region around the decision boundary. We utilize k nearest neighbors to look around the pattern's periphery. The first neighborhood property is that "a pattern located near the decision boundary tends to have more heterogeneous neighbors in their class membership." The second neighborhood property dictates that "a noisy pattern tends to belong to a different class from that of its neighbors." And the third neighborhood property is that "the neighbors of the decision boundary pattern tend to be located near the decision boundary as well." The first property is used for identifying the patterns located near the decision boundary. The second property is used for removing the patterns located on the wrong side of the decision boundary. And the third property is used for skipping unnecessary distance calculation, thus accelerating the pattern selection procedure. The letter also provides how to choose k for the

proposed algorithm. Note that it has been skipped or dealt with as trivial in other pattern selection methods that employ either k-means clustering or the k-nearest neighbor rule.

The remaining part of this letter is organized as follows. Section 2 briefly explains the SVM theory, in particular, the patterns critically affecting the training. Section 3 presents the proposed method, NPPS, that selects the patterns near the decision boundary. Section 4 explains how to choose the number of neighbors, k—the parameter of the proposed method. Section 5 provides the experimental results on artificial data sets, real-world bench-marking data sets, and a real-world marketing data set. We conclude with some future work in section 6.

2 Support Vector Machines and Critical Training Patterns

Support vector machines (SVMs) are a general class of statistical learning architectures that perform structural risk minimization on a nested set structure of separating hyperplanes (Cristianini & Shawe-Taylor, 2000; Schölkopf & Smola, 2002; Vapnik, 1999). Consider a binary classification problem with M patterns $(\vec{x}_i, y_i), i = 1, \ldots, M$ where $\vec{x}_i \in \Re^d$ and $y_i \in \{-1, 1\}$. Let us assume that patterns with $y_i = 1$ belong to class 1, while those with $y_i = -1$ belong to class 2. SVM training involves solving the following quadratic programming problem, which yields the largest margin ($\frac{2}{\|w\|}$) between classes.

$$\begin{aligned} \min \quad & \Theta(\vec{w}, \xi) = \frac{1}{2}||\vec{w}||^2 + C\sum_i^M \xi_i, \\ \text{s. t.} \quad & y_i\,(\vec{w} \cdot \Phi(\vec{x}_i) + b) \geq 1 - \xi_i, \\ & \xi_i \geq 0, \quad i = 1, \ldots, M, \end{aligned} \tag{2.1}$$

where $\vec{w} \in \Re^d, b \in \Re$ (see Figure 1, and an error tolerance parameter $C \in \Re$. Equation 2.1 is the most general SVM formulation, allowing both nonseparable and nonlinear cases. The ξ's are nonnegative slack variables, which play a role of allowing a certain level of misclassification for a nonseparable case. The $\Phi(\cdot)$ is a mapping function for a nonlinear case that projects patterns from the input space into a feature space. This nonlinear mapping is performed implicitly by employing a kernel function $K(\vec{x}, \vec{x}')$ to avoid the costly calculation of inner products, $\Phi(\vec{x}) \cdot \Phi(\vec{x})$.[1] There are three typical

[1] Aside from the computational efficiency by dot-product replacement, the kernels provide operational benefits as well: it is easy and natural to work on (or integrate) various types of data—vectors, sequences, text, images, and graphs, for example—and to detect very general types of relations therein.

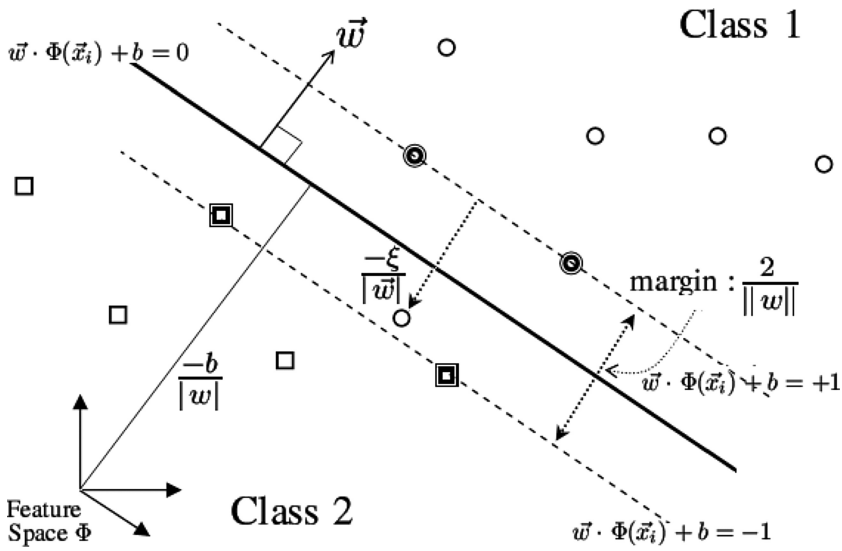


Figure 1: SVM classification problem: Through a mapping function $\Phi(\cdot)$, the class patterns are linearly separated in a feature space. The patterns determining both margin hyperplanes are outlined. The decision boundary is the halfway hyperplane between margins.

kernel functions: RBF, polynomial, and sigmoid in due order,

$$\begin{aligned} K(\vec{x}, \vec{x}') &= exp(-||\vec{x} - \vec{x}'||^2/2\sigma^2), \\ K(\vec{x}, \vec{x}') &= (\vec{x} \cdot \vec{x}' + 1)^p, \\ K(\vec{x}, \vec{x}') &= \tanh(\rho(\vec{x} \cdot \vec{x}') + \delta). \end{aligned} \tag{2.2}$$

The optimal solution of equation 2.1 yields a decision function of the following form,

$$\begin{aligned} f(\vec{x}) &= sign(\vec{w} \cdot \Phi(\vec{x}) + b) = sign\left(\sum_{i=1}^{M} y_i \alpha_i \Phi(\vec{x}_i) \cdot \Phi(\vec{x}) + b\right) \\ &= sign\left(\sum_{i=1}^{M} y_i \alpha_i K(\vec{x}_i, \vec{x}) + b\right), \end{aligned} \tag{2.3}$$

where α_is are nonnegative Lagrange multipliers associated with training patterns, respectively. The solutions, α_is, are obtained from the dual problem of equation 2.1, which minimizes the convex quadratic objective

function under constraints

$$\min_{0\le\alpha_i\le C} W(\alpha_i, b) = \frac{1}{2}\sum_{i,j=1}^{M}\alpha_i\alpha_j y_i y_j K(\vec{x}_i\cdot\vec{x}_j) - \sum_{i=1}^{M}\alpha_i + b\sum_{i=1}^{M} y_i\alpha_i.$$

The first-order conditions on $W(\alpha_i, b)$ are reduced to the Karush-Kuhn-Tucker (KKT) conditions,

$$\frac{\partial W(\alpha_i, b)}{\partial\alpha_i} = \sum_{j=1}^{M} y_i y_j K(\vec{x}_i, \vec{x}_j)\alpha_j + y_i b - 1 = y_i\bar{f}(\vec{x}_i) - 1 = g_i,$$

$$\frac{\partial W(\alpha_i, b)}{\partial b} = \sum_{j=1}^{M} y_j\alpha_j = 0, \tag{2.4}$$

where $\bar{f}(\cdot)$ is the function inside the parentheses of *sign* in equation 2.3. The KKT complementarity condition, equation 2.4, partitions the training pattern set into three categories according to the corresponding α_is:

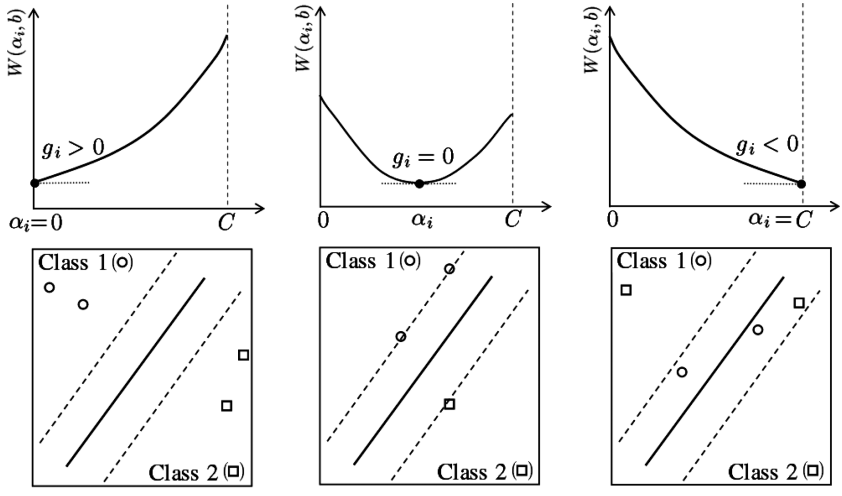
(a) $g_i > 0 \quad\rightarrow\quad \alpha_i = 0 \qquad$: irrelevant patterns

(b) $g_i = 0 \quad\rightarrow\quad 0 < \alpha_i < C$: margin support vectors

(c) $g_i < 0 \quad\rightarrow\quad \alpha_i = C \qquad$: error support vectors

Figure 2 illustrates those categories (Cauwenberghs & Poggio, 2001; Pontil & Verri, 1998). The patterns belonging to category a are out of the margins, thus irrelevant to training, while the patterns belonging to categories b and c are critical and directly affect training. They are called support vectors (SVs). The patterns of category b are strictly on the margin; hence, they are called *margin SVs*. The patterns of category c lie between two margins; hence, they are called *error SVs* but are not necessarily misclassified. (Note that there is another type of SV belonging to the category of error SV. They are incorrectly labeled patterns that could be located very far from the decision boundary. We regard them as outliers that do not contribute to margin construction. We focus only on the SVs located around the decision boundary, not those located deep in the realm of the opposite class.) Going back to equation 2.3, we can now see that the decision function is a linear combination of kernels on only those critical training patterns (denoted as SVs) because the patterns corresponding to $\alpha_i = 0$ have no influence on the decision result:

$$f(\vec{x}) = sign\left(\sum_{i=1}^{M} y_i\alpha_i K(\vec{x}_i, \vec{x}) + b\right) = sign\left(\sum_{i\in\mathbf{SVs}} y_i\alpha_i K(\vec{x}_i, \vec{x}) + b\right). \tag{2.5}$$



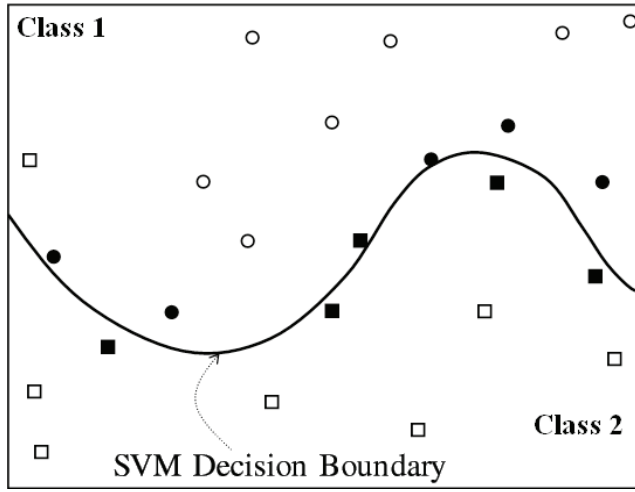
a. Non SVs b. Margin SVs c. Error SVs

Figure 2: Three categories of training patterns.

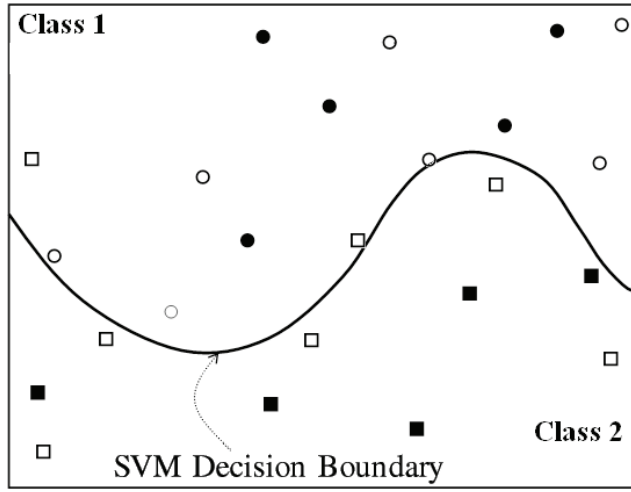
Equation 2.5 leads us to an attempt that reduces the whole training set to a subset of would-be SVs.

3 Neighborhood Property–Based Pattern Selection

To circumvent memory- and time-demanding SVM training, we propose a preprocessing algorithm: a neighborhood property–based pattern selection algorithm (NPPS). The idea of the algorithm is to select only those patterns located around the decision boundary since they are the ones that contain the most information. Contrary to a usually employed random sampling, this approach can be viewed as informative or intelligent sampling. Figure 3 conceptually shows the difference between NPPS and random sampling in selecting a subset of the training data. NPPS selects the patterns in the region around the decision boundary, and random sampling selects those from the whole input space. Obviously no one knows how close a pattern is to the decision boundary until a classifier is built. However, we can infer the proximity ahead of training by utilizing neighborhood properties. The first neighborhood property is that "a pattern located near the decision boundary tends to have more heterogeneous neighbors in its class membership." A well-known entropy concept can be utilized for the measurement of heterogeneity of class labels among k-nearest neighbors. And the measure will lead us to estimate the proximity accordingly. Here, we define a measure



a. NPPS



b. Random Sampling

Figure 3: NPPS and random sampling select different subsets. Open circles and squares are the patterns belonging to class 1 and class 2, respectively. Filled circles and squares are the selected patterns.

by using (negative) entropy,

$$\text{Neighbors\_Entropy}\ (\vec{x}, k) = \sum_{j=1}^{J} P_j \cdot \log_J \frac{1}{P_j},$$

where j indicates a particular class out of J classes, and P_j is defined as k_j/k, where k_j is the number of the neighbors belonging to class j. In most cases, a pattern with a positive value of Neighbors_Entropy $(\vec{x}, k)$ is close to the decision boundary, and thus selected. Those patterns are likely to be SVs, which correspond to the margin SVs in Figure 2b or the error SVs in Figure 2c. Among the patterns having a positive value of Neighbors_Entropy $(\vec{x}, k)$, noisy patterns are also present. Here, let us define an overlap region as a hypothetical region in feature space shared by both classes, and overlap patterns as the patterns in that region. (We defer the finer definitions for overlap region and overlap patterns until section 4.1). A set of overlap patterns contains the patterns located not only on the right side of the decision boundary but also on the other side of it. The latter denotes noisy patterns, which should be identified and removed as much as possible because they are more likely to be the error SVs that would be misclassified. To remove this noisy pattern, we take the second neighborhood property: An overlap pattern or an outlier tends to belong to a different class from its neighbors. If a pattern's own label is different from the majority label of its neighbors, it is likely to be incorrectly labeled. The measure Neighbors_Match $(\vec{x}, k)$ is defined as the ratio of neighbors whose label matches that of $\vec{x}$,

$$\text{Neighbors\_Match}\ (\vec{x}, k) = \frac{|\{\vec{x}' | label(\vec{x}') = label(\vec{x}),\ \vec{x}' \in kNN(\vec{x})\}|}{k},$$

where $kNN(\vec{x})$ is the set of k nearest neighbors of $\vec{x}$. The patterns with a small Neighbors_Match $(\vec{x}, k)$ value are likely to be the ones incorrectly labeled. In that point of view, Neighbors_Match can be interpreted as a confidence for k-nearest neighbor classification. Only the patterns satisfying the two conditions, Neighbors_Entropy $(\vec{x}, k) > 0$ and Neighbors_Match $(\vec{x}, k) \geq \frac{1}{J}$, are selected.

Figure 4 shows a toy example of how patterns are selected by the proposed measures. The numbers scattered in the figure (1, 2, and 3) stand for the class labels of the patterns. We assume $J = 3$ and $k = 6$. For representational simplicity, we consider only six patterns marked by dotted circles. Table 1 presents the values of P_j, Neighbors_Entropy, and Neighbors_Match for these marked patterns. Let us consider $\vec{x}^1$ first. $\vec{x}^1$ is remote from the decision boundary belonging to class 1 and is thus surrounded by the neighbors belonging to class 1. $\vec{x}^1$ is not selected since it does not satisfy the condition of Neighbors_Entropy. Meanwhile, $\vec{x}^2$ resides in a deep region

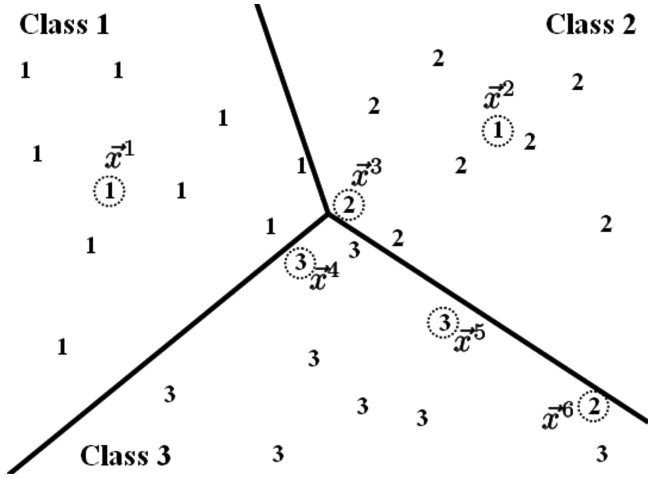


Figure 4: A toy example. The numbers scattered in the figure (1, 2, and 3) stand for the class labels of the patterns. The parameters are assumed to be $J = 3$ and $k = 6$. For representational simplicity, we consider only 6 patterns (out of 29) marked by dotted circles. Table 1 shows the patterns selected by the proposed measures presenting details: the values of P_j, Neighbors_Entropy, and Neighbors_Match.

of class 2, but it is a noise pattern labeled as class 1. Since the composition of class membership of its neighbors is homogeneous (all of them belong to class 2), it also has a zero value of Neighbors_Entropy. Therefore, it is excluded from selection. However, the case of the pattern $\vec{x}^2$ is different from the case of the pattern $\vec{x}^1$; for the pattern $\vec{x}^2$, all its neighbors belong to a different class from the class of $\vec{x}^2$, while for the pattern $\vec{x}^1$, all its neighbors belong to the same class that $\vec{x}^1$ belongs to. We can differentiate two cases by Neighbors_Match, which is 1 for $\vec{x}^1$ and 0 for $\vec{x}^2$. In any case, the remote patterns from the decision boundary are screened out by the proposed measures. On the other hand, the pattern $\vec{x}^3$ is close to the decision boundary, and the composition of the neighbors shows heterogeneous class membership; two of them belong to class 1, another two belong to class 2, and the rest belong to class 3. This leads to Neighbors_Entropy = 1 and Neighbors_Match = 1/3, and consequently satisfies the conditions. Similarly, the patterns $\vec{x}^4$ and $\vec{x}^5$ are chosen. From the example, we can see that the selected patterns are distributed near the decision boundary and almost correctly labeled.

However, NPPS takes $O(M^2)$ to evaluate kNNs for M patterns, so the pattern selection process itself can be time-consuming. To accelerate the pattern selection procedure, we consider the third neighborhood property: The neighbors of a pattern located near the decision boundary tend to be

Table 1: A Toy Example: Patterns Selected by Neighbors_Entropy and Neighbors_Match.

		Class Labels of Neighbors											
	j^*	j^1	j^2	j^3	j^4	j^5	j^6	P_1	P_2	P_3	Neighbors_Entropy	Neighbors_Match	Selected Patterns
$\vec{x}^1$	1	1	1	1	1	1	1	6/6	0/6	0/6	0	6/6	X
$\vec{x}^2$	1	2	2	2	2	2	2	0/6	6/6	0/6	0	0/6	X
$\vec{x}^3$	2	1	1	2	2	3	3	2/6	2/6	2/6	1	2/6	◯
$\vec{x}^4$	3	3	3	2	2	3	1	1/6	2/6	3/6	0.9227	3/6	◯
$\vec{x}^5$	3	3	3	3	3	3	2	0/6	1/6	5/6	0.4100	5/6	◯
$\vec{x}^6$	2	3	3	3	3	3	2	0/6	1/6	5/6	0.4100	1/6	X

Notes: j^* is the class label of pattern $\vec{x}^i$, and j^k is the label of its kth nearest neighbor. Refer to Figure 4.

NPPS (D, k) {

[**0**] Initialize $\mathbf{D}_\mathbf{e}^0$ with randomly chosen patterns from $\mathbf{D}$.

Constants, k and J, are given. Initialize i and various sets as follows:

$$i \leftarrow 0, \quad \mathbf{S}_\mathbf{o}^0 \leftarrow \emptyset, \quad \mathbf{S}_\mathbf{x}^0 \leftarrow \emptyset, \quad \mathbf{S}^0 \leftarrow \emptyset.$$

while $\mathbf{D}_\mathbf{e}^i \neq \emptyset$ **do**

[**1**] Choose $\vec{x}$ satisfying [Expanding Criteria].

$$\mathbf{D}_\mathbf{o}^i \leftarrow \{\vec{x} \mid \mathrm{Neighbors\_Entropy}(\vec{x}; \mathrm{k}) > 0,\ \vec{x} \in \mathbf{D}_\mathbf{e}^i\}.$$

$$\mathbf{D}_\mathbf{x}^i \leftarrow \mathbf{D}_\mathbf{e}^i - \mathbf{D}_\mathbf{o}^i.$$

[**2**] Select $\vec{x}$ satisfying [Selecting Criteria].

$$\mathbf{D}_\mathbf{s}^i \leftarrow \{\vec{x} \mid \mathrm{Neighbors\_Match}(\vec{x}; \mathrm{k}) \geq 1/J,\ \vec{x} \in \mathbf{D}_\mathbf{o}^i\}.$$

[**3**] Update the pattern sets.

$$\mathbf{S}_\mathbf{o}^{i+1} \leftarrow \mathbf{S}_\mathbf{o}^i \cup \mathbf{D}_\mathbf{o}^i \text{ : the expanded,}$$

$$\mathbf{S}_\mathbf{x}^{i+1} \leftarrow \mathbf{S}_\mathbf{x}^i \cup \mathbf{D}_\mathbf{x}^i \text{ : the nonexpanded,}$$

$$\mathbf{S}^{i+1} \leftarrow \mathbf{S}^i \cup \mathbf{D}_\mathbf{s}^i \text{ : the selected.}$$

[**4**] Compute the next evaluation set $\mathbf{D}_\mathbf{e}^{i+1}$.

$$\mathbf{D}_\mathbf{e}^{i+1} \leftarrow \bigcup_{\vec{x} \in \mathbf{D}_\mathbf{o}^i} k\mathbf{NN}(\vec{x}) - (\mathbf{S}_\mathbf{o}^{i+1} \cup \mathbf{S}_\mathbf{x}^{i+1}).$$

[**5**] $i \leftarrow i + 1$.

end

return $\mathbf{S}^i$

}

Figure 5: NPPS algorithm.

Table 2: Notation.

Symbol	Meaning
$\mathbf{D}$	The original training set whose cardinality is M
$\mathbf{D}_{\mathbf{e}}^{i}$	The evaluation set at ith step
$\mathbf{D}_{\mathbf{o}}^{i}$	A subset of $\mathbf{D}_{\mathbf{e}}^{i}$, the set of patterns to be expanded from $\mathbf{D}_{\mathbf{e}}^{i}$, each element of which will compute its k nearest neighbors to constitute the next evaluation set, $\mathbf{D}_{\mathbf{e}}^{i+1}$
$\mathbf{D}_{\mathbf{x}}^{i}$	A subset of $\mathbf{D}_{\mathbf{e}}^{i}$, the set of patterns not to be expanded from $\mathbf{D}_{\mathbf{e}}^{i}$, or $\mathbf{D}_{\mathbf{x}}^{i} = \mathbf{D}_{\mathbf{e}}^{i} - \mathbf{D}_{\mathbf{o}}^{i}$
$\mathbf{D}_{\mathbf{s}}^{i}$	The set of "selected" patterns from $\mathbf{D}_{\mathbf{o}}^{i}$ at ith step
$\mathbf{S}_{\mathbf{o}}^{i}$	The accumulated set of expanded patterns, $\bigcup_{j=0}^{i-1} \mathbf{D}_{\mathbf{o}}^{j}$
$\mathbf{S}_{\mathbf{x}}^{i}$	The accumulated set of nonexpanded patterns, $\bigcup_{j=0}^{i-1} \mathbf{D}_{\mathbf{x}}^{j}$
$\mathbf{S}^{i}$	The accumulated set of selected patterns, $\bigcup_{j=0}^{i-1} \mathbf{D}_{\mathbf{s}}^{j}$ the last of which $\mathbf{S}^{N}$ is the reduced training pattern set
$k\mathbf{NN}(\vec{x})$	The set of k nearest neighbors of $\vec{x}$

located near the decision boundary as well. Assuming the property, one may narrow the scope of computation from all the training patterns to the patterns near the decision boundary. Only the neighbors of a pattern satisfying Neighbors_Entropy $(\vec{x}, k) > 0$ are evaluated in the next step. This lazy evaluation can reduce the practical time complexity from $O(M^2)$ to $O(vM)$, where v is the number of patterns in the overlap region. In most practical problems, $v < M$ holds. In addition, any algorithm on efficient nearest-neighbor searching can be incorporated into the proposed method to further reduce the time complexity. There is a considerable amount of literature about efficient searching for nearest neighbors. Some of it attempts to save distance computation time (Grother, Candela, & Blue, 1997; Short & Fukunaga, 1981), and others attempt to avoid redundant searching time (Bentley, 1975; Friedman, Bentley, & Finkel, 1977; Guttman, 1984; Masuyama, Kudo, Toyama, & Shimbo, 1999). Apart from them, there are many sophisticated NN classification algorithms such as approximated (Arya, Mount, Netanyahu, Silverman, & Wu, 1998; Indyk, 1998), *condensed* (Hart, 1968), and *reduced* (Gates, 1972). (See also Berchtold, Böhm, Keim, & Kriegel, 1997; Borodin, Ostrovsky, & Rabani, 1999; Ferri, Albert, & Vidal, 1999; Johnson, Ladner, & Riskin, 2000; Kleingberg, 1997; Tsaparas, 1999.)

The time complexity analysis for the fast NPPS can be found online at http://www.kyb.mpg.de/publication.html?user=shin and Shin and Cho (2003a), and a brief empirical result in appendix A. The algorithm and related notations are shown in Figure 5 and Table 2.

4 How to Determine the Number of Neighbors

In this section, we briefly introduce a heuristic for determining the value of k. Too large a value of k results in too many patterns being selected.

Consequently, we will achieve little effect of pattern selection. Too small a value of k, leads to few patterns selected. However, it may degrade SVM accuracy since there are more chances to miss important patterns—the would-be support vectors. The dilemma about k will not be symmetrical because a serious loss of accuracy is not likely to be well compensated for by the benefit of a downsized training set. This point relates to our idea: the selected pattern set should be large enough to contain at least the patterns in the overlap region. Therefore, we must first estimate how many training patterns reside in the overlap region. Based on the estimate, the next step is to enlarge the value of k until the size of the corresponding set covers the estimate. Under this condition, the minimum value of k will be regarded as optimal unless SVM accuracy degrades.

In the following sections, we first identify the overlap region **R** and the overlap set **V**. Second, we estimate the lower bound on the cardinality of **V**. Third, we define Neighbors_Entropy set $\mathbf{B}_k$ with respect to the value of k and some related properties as well. Finally, we provide a systematic procedure for determining the value of k.

4.1 Overlap Region and Overlap Set. Consider a two-class classification problem (see Figure 6),

$$f(\vec{x}) = \begin{cases} \vec{x} \rightarrow C_1 & \text{if} \quad f(\vec{x}) > 0, \\ \vec{x} \rightarrow C_2 & \text{if} \quad f(\vec{x}) < 0, \end{cases} \tag{4.1}$$

where $f(\vec{x})$ is a classifier and $f(\vec{x}) = 0$ is the decision boundary. Let us define noisy overlap patterns (NOPs) as the patterns that are located on the wrong side of the decision boundary. They are shown in Figure 6 as squares located above $f(\vec{x}) = 0$ and circles located below $f(\vec{x}) = 0$. Let **R** denote the overlap region—a hypothetical region where NOPs reside, the convex-hull of NOPs, enclosed by the dotted lines in Figure 6. Similarly, let us define *correct overlap patterns* (COPs) as the patterns that are enveloped by the convex hull, yet in the right class side. Note that **R** is defined by NOPs, but it contains not only NOPs but also COPs. Let **V** denote the overlap set defined as the intersection of **D** and **R** (that is, the subset of **D** that comprises NOPs and COPs. There are six NOPs and six COPs in Figure 6. The cardinality of **V** is denoted as v.

4.2 Size Estimation of Overlap Set. Now we estimate v. Let $P_{\mathbf{R}}(\vec{x})$ denote the probability that a pattern $\vec{x}$ falls in the region **R**. Then we can calculate the expected value of v from the given training set **D** as

$$v = MP_{\mathbf{R}}(\vec{x}), \tag{4.2}$$

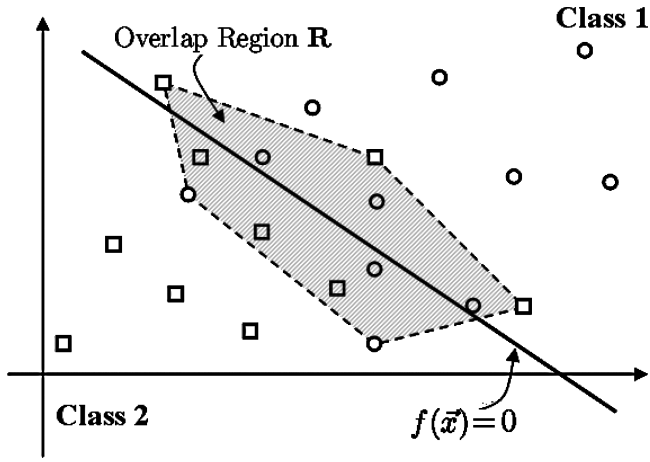


Figure 6: Two-class classification problem where the circles belong to class 1 and the squares belong to class 2. The area enclosed by the dotted lines is defined as overlap region **R**. The area comprises the overlap set **V** of NOPs and COPs.

where M is the number of the training patterns, say, $M = |\mathbf{D}|$. The probability $P_{\mathbf{R}}(\vec{x})$ can be dissected class-wise, such as

$$P_{\mathbf{R}}(\vec{x}) = \sum_{j=1}^{2} P(\vec{x} \in \mathbf{R}, C_j), \tag{4.3}$$

where $P(\vec{x} \in \mathbf{R}, C_j)$ is the joint probability of $\vec{x}$ belonging to class C_j and lying in **R**. Note that $P_{\mathbf{R}}(\vec{x})$ also can be interpreted as the probability of $\vec{x}$ being COPs or NOPs. Further, if the region **R** is divided into

$$\mathbf{R}_1 = \{\vec{x} \in \mathbf{R} \mid f(\vec{x}) \geq 0\} \text{ and } \mathbf{R}_2 = \{\vec{x} \in \mathbf{R} \mid f(\vec{x}) < 0\}, \tag{4.4}$$

Equation 4.3 can be rewritten as

$$\begin{aligned} P_{\mathbf{R}}(\vec{x}) &= P(\vec{x} \in \mathbf{R}, C_1) + P(\vec{x} \in \mathbf{R}, C_2) \\ &= P(\vec{x} \in \mathbf{R}_1 \cup \mathbf{R}_2, C_1) + P(\vec{x} \in \mathbf{R}_1 \cup \mathbf{R}_2, C_2) \\ &= \underbrace{\left\{P(\vec{x} \in \mathbf{R}_1, C_2) + P(\vec{x} \in \mathbf{R}_2, C_1)\right\}}_{\textbf{(a)}} \\ &\quad + \underbrace{\left\{P(\vec{x} \in \mathbf{R}_1, C_1) + P(\vec{x} \in \mathbf{R}_2, C_2)\right\}}_{\textbf{(b)}}. \end{aligned} \tag{4.5}$$

In the last row, a and b denote the probabilities of the patterns located in $\mathbf{R}$ that are incorrectly and correctly classified—NOPs and COPs, respectively. Since all NOPs are the incorrectly classified patterns, a can be estimated from the misclassification error rate P_{error} of the classifier $f(\vec{x})$. On the contrary, it is not easy to estimate b.[2] Therefore, what we can do in practice is to infer the lower bound of it. Generally: the following inequality holds,

$$P(\vec{x} \in \mathbf{R}_j, C_j) \geq P(\vec{x} \in \mathbf{R}_j, C_i), \quad j \neq i. \tag{4.6}$$

Based on that, equation 4.5 can be simplified as

$$P_{\mathbf{R}}(\vec{x}) \geq 2P_{error}, \tag{4.7}$$

and the lower bound of v becomes

$$v \;\geq\; v^{LOW} = 2MP_{error} \tag{4.8}$$

from equation 4.2.

4.3 Pattern Set with Positive Neighbors_Entropy. Let us define $\mathbf{B}_k$ given a specified value of k,

$$\mathbf{B}_k = \{\vec{x} \mid \text{Neighbors\_Entropy}(\vec{x}, k) > 0,\ \vec{x} \in \mathbf{D}\}. \tag{4.9}$$

Note that $\mathbf{B}_k$ is the union of $\mathbf{D}_{\mathbf{o}}^i$'s, $\mathbf{B}_k = \bigcup_{i=0}^{N} \mathbf{D}_{\mathbf{o}}$ where N is the total number of iterations in the algorithm NPPS (see Figure 5). The following property of $\mathbf{B}_k$ leads to a simple procedure.

Lemma 1. *A Neighbors_Entropy set* $\mathbf{B}_k$ *is a subset of* $\mathbf{B}_{k+1}$*:*

$$\mathbf{B}_k \subseteq \mathbf{B}_{k+1} \quad 2 \leq k \leq M-2. \tag{4.10}$$

Proof. Denote P_j^k as the probability that k_j out of k nearest neighbors belong to class C_j. If $\vec{x} \in \mathbf{B}_k$, then it means Neighbors_Entropy $(\vec{x}, k) > 0$. A positive Neighbors_Entropy is always accompanied by $P_j^k = \frac{k_j}{k} < 1,\ \forall j$. Therefore,

$$k_j < k,\ \forall j.$$

[2] Of course, if $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ contain roughly the same number of correct and incorrect patterns, the probabilities of a and b become similar. But this assumption will work only when both class distributions follow the uniform distribution.

Adding 1 to both sides yields

$$(k_j + 1) < (k + 1), \ \forall j.$$

Suppose the $(k+1)^{\text{th}}$ nearest neighbor of $\vec{x}$ belongs to C_{j^*}. Then $(k_{j^*} + 1) < (k + 1)$ holds for j^*, while $k_j < (k + 1)$ holds for $j \neq j^*$. The inequalities lead to $P_{j^*}^{k+1} < 1$ and $P_{j \neq j^*}^{k+1} < 1$, respectively. As a consequence, we have a positive Neighbors_Entropy of $\vec{x}$ in the case of the $(k+1)^{\text{th}}$ nearest neighbor as well. Therefore, Neighbors_Entropy $(\vec{x}, k + 1) > 0$, which indicates $\vec{x} \in \mathbf{B}_{k+1}$.

From lemma 1, it follows that b_k, the cardinality of $\mathbf{B}_k$, is an increasing function of k.

4.4 Procedure for Determining the Number of Neighbors. $\mathbf{B}_k$ larger than $\mathbf{V}$ merely increases the SVM training time by introducing redundant training patterns. In contrast, $\mathbf{B}_k$ smaller than $\mathbf{V}$ could degrade the SVM accuracy. Therefore, our objective is to find the smallest $\mathbf{B}_k$ that covers $\mathbf{V}$.

Let us define $k^{\min}$ using the lower bound of v from equation 4.8:

$$k^{\min} = \min \{k \mid b_k \geq v^{LOW}, \ \ k \geq 2 \}.$$

From lemma 1, we know that b_k is an increasing function of k. Therefore, it is not necessary to evaluate the values of k less than $k^{\min}$. Instead, we check the stabilization of SVM training error rate P_{error}^{svm} only for the k's larger than $k^{\min}$ by increasing the value little by little. The optimal value of k is then chosen as

$$k^* = \arg\min \{ \ |P_{error}^{svm}(k) - P_{error}^{svm}(k+1)| \leq \epsilon, \ k \geq k^{\min}\}, \tag{4.11}$$

where ϵ is set to a trivial value. Eauation 4.11 requires several dry runs of SVM training. However, the runs are not likely to impose heavy computational burden since the strong inequality $b_k << M$ holds for the first smallest k's, and hence the size of the training set (the selected pattern set) is small. The procedure is summarized in Figure 7.[3] The main contribution of the proposed procedure is to limit the search space of k by means of the lower-bound estimation of the size of overlap set. More details can be found in Shin and Cho (2003b) and some empirical results in appendix B.

[3] There are several benefits of using *1*-NN rule as a P_{error} estimator in step 1 since it is a local learning algorithm, simple, and computationally efficient. One can skip step 1 if an approximate P_{error} of the problem is given a priori.

[**1**] Estimate P_{error}:

$\hat{P}_{error}$ is calculated based on the training error rate of *1*-NN rule.

[**2**] Calculate the lower bound of v according to equation 4.8:

$$v \geq \quad v^{LOW} = 2M\hat{P}_{error}.$$

[**3**] Find k^* according to equation 4.11:

$$k^* = \arg\min \{\ |P^{svm}_{error}(k) - P^{svm}_{error}(k+1)| \leq \epsilon,\ k \geq k^{\min}\}.$$

where $k^{\min} = \min \{k \mid b_k \geq v^{LOW},\ \ k \geq 2\ \}$

and ϵ is a trivial value.

Figure 7: Procedure to determine the value of k.

5 Experiments

We applied NPPS to various kinds of data sets: artificial data sets, benchmarking data sets, and a real-world marketing data set. The following three sections present the experimental results in order.

5.1 Artificial Data Sets. The first problem was drawn from four gaussian densities: the continuous XOR problem. A total of 600 training patterns, 300 from each class, were generated. The classes, C_1 and C_2, were defined as

$$C_1 = \left\{\vec{x} \mid \vec{x} \in N_{1A} \cup N_{1B},\ \begin{bmatrix}-3\\-3\end{bmatrix} \leq \vec{x} \leq \begin{bmatrix}3\\3\end{bmatrix}\right\},$$
$$C_2 = \left\{\vec{x} \mid \vec{x} \in N_{2A} \cup N_{2B},\ \begin{bmatrix}-3\\-3\end{bmatrix} \leq \vec{x} \leq \begin{bmatrix}3\\3\end{bmatrix}\right\},$$

where

$$N_{1A} = \left\{\vec{x}|N\left(\begin{bmatrix}1\\1\end{bmatrix}, \begin{bmatrix}0.5^2 & 0\\0 & 0.5^2\end{bmatrix}\right)\right\}, N_{1B} = \left\{\vec{x}|N\left(\begin{bmatrix}-1\\-1\end{bmatrix}, \begin{bmatrix}0.5^2 & 0\\0 & 0.5^2\end{bmatrix}\right)\right\},$$
$$N_{2A} = \left\{\vec{x}|N\left(\begin{bmatrix}-1\\1\end{bmatrix}, \begin{bmatrix}0.5^2 & 0\\0 & 0.5^2\end{bmatrix}\right)\right\}, N_{2B} = \left\{\vec{x}|N\left(\begin{bmatrix}1\\-1\end{bmatrix}, \begin{bmatrix}0.5^2 & 0\\0 & 0.5^2\end{bmatrix}\right)\right\}.$$

See also Figure 11.1a. The second problem is the sine function problem. The input patterns were generated from a two-dimensional uniform distribution, and then the class labels were determined by whether the pattern was located above or below a sine decision function:

$$C_1 = \left\{ \vec{x} \mid x_2 > \sin(3x_1 + 0.8)^2, \begin{bmatrix} 0 \\ -2.5 \end{bmatrix} \leq \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \leq \begin{bmatrix} 1 \\ 2.5 \end{bmatrix} \right\}$$

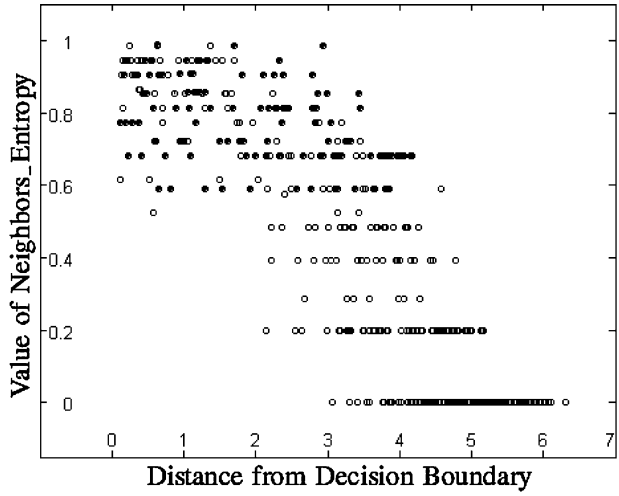
$$C_2 = \left\{ \vec{x} \mid x_2 \leq \sin(3x_1 + 0.8)^2, \begin{bmatrix} 0 \\ -2.5 \end{bmatrix} \leq \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \leq \begin{bmatrix} 1 \\ 2.5 \end{bmatrix} \right\}.$$

To make the density near the decision boundary thicker, four different gaussian noises were added along the decision boundary: $N(\vec{\mu}, s^2 I)$ where $\vec{\mu}$ is an arbitrary point on the decision boundary and s is a gaussian width parameter ($s = 0.1,\ 0.3,\ 0.8,\ 1.0$). A total of 500 training patterns were generated including noises. Figure 11.1b shows the problem.

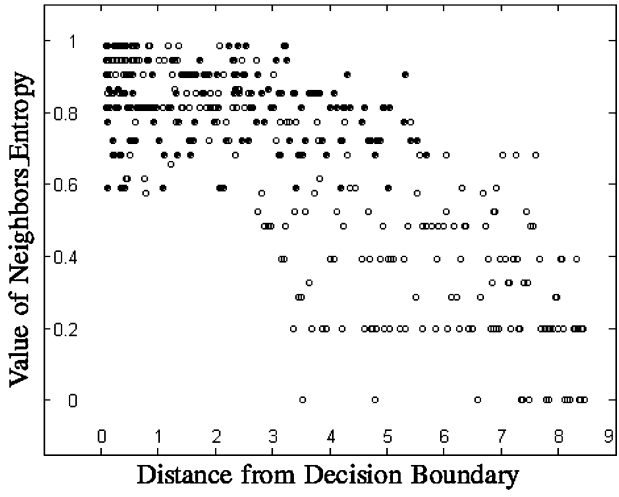
For both problems, Figure 8 presents the relationship between distance from decision boundary to a pattern and its value of Neighbors_Entropy. The closer to the decision boundary a pattern is, the higher the value of Neighbors_Entropy it has. Both Figures 8a and 8b ensure that Neighbors_Entropy is pertinent to estimating the proximity to the decision boundary. Among the patterns with positive Neighbors_Entropy values, the ones that meet the Neighbors_Match condition are selected. They are depicted as filled circles against open ones. Note that the filled circles are distributed nearer the decision boundary. The distribution of the selected patterns is shown in Figures 11.3a and 11.3b.

NPPS changes the size as well as the distribution of the training set. Such changes may change the optimal value of hyperparameter that brings the best result. Thus, we first observed the effect of change of training set. The SVM performance was measured under various combinations of hyperparameters such as $(C, \sigma) \in \{0.1, 1.0, 10, 100, 1000\} \times \{0.25, 0.5, 1, 2, 3\}$, where C and σ indicate misclassification tolerance and gaussian kernel width, respectively. For each of the artificial problems, 1000 test patterns were generated from the statistically identical distributions to its original training set. We compared the test error rates (%) of SVM when trained with all patterns (ALL), trained with random patterns (RAN), and trained with the selected patterns (SEL).

Figure 9 depicts the test error rate over the hyperparameter variation for Continuous XOR problem. The most pronounced feature is the higher sensitivity of SEL to hyperparameter variation than before (ALL). It may be caused by the fact that the patterns selected by NPPS are mostly distributed in the narrow region along the decision boundary. In Figure 9a, for instance, SEL shows a sudden rise of the test error rate for σ larger than a certain value when C is fixed, and similarly, a sharp descent after a certain value of C when σ is fixed. An interesting point is that SEL can always reach

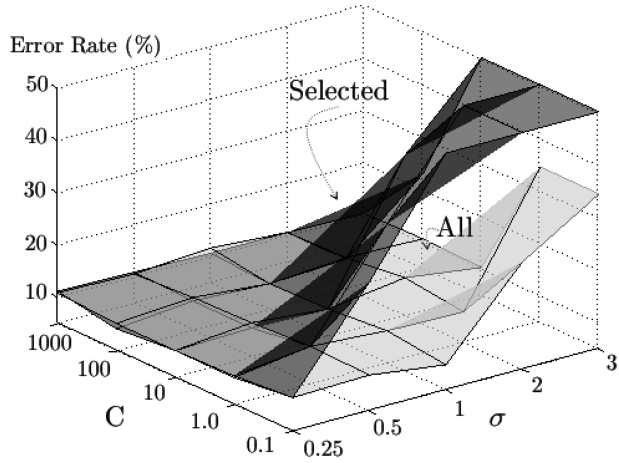


a. Continuous XOR problem

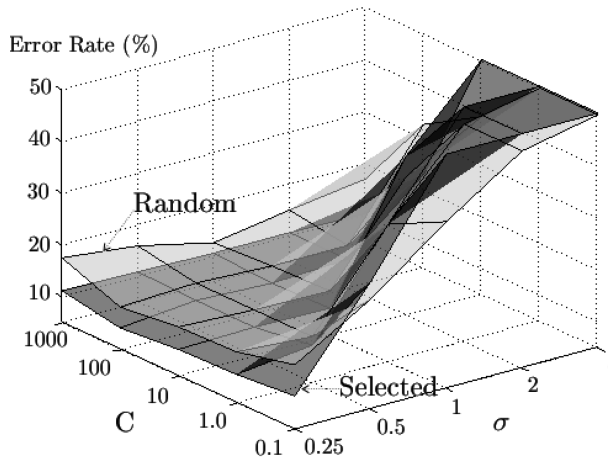


b. Sine Function problem

Figure 8: The relationship between the distance from decision boundary and Neighbors_Entropy. The closer to decision boundary a pattern is, the higher value of Neighbors_Entropy it has. The selected patterns are depicted as filled circles against open ones.



a. SEL VS. ALL



b. SEL VS. RAN

Figure 9: Performance comparison over hyperparameter variation: Continuous XOR problem.

a performance comparable to that of ALL by adjusting the value of the hyper-parameters. Now we compare SEL and RAN from Figure 9b. We used the same number of random samples as that of the patterns selected by NPPS. Therefore, there is no difference in the size of training set, only a difference in data distribution. When compared with SEL, RAN is less

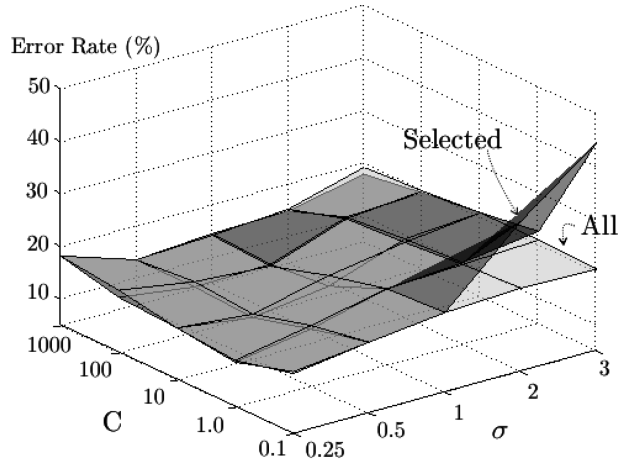
Table 3: Best Result Comparison: ALL vs. RAN vs. SEL.

	Continuous XOR			Sine Function		
(C, σ)	ALL (10, 0.5)	RAN (100, 1)	SEL (100, 0.25)	ALL (10, 0.5)	RAN (0.1, 0.25)	SEL (10, 0.5)
Execution time (sec)	454.83	3.02	3.85	267.76	8.97	8.79
Number of training patterns	600	180	180	500	264	264
Number of support vectors	167	68	84	250	129	136
Test error (%)	9.67	12.33	9.67	13.33	16.34	12.67
McNemar's test (p-value)	—	0.08	1.00	—	0.12	0.89

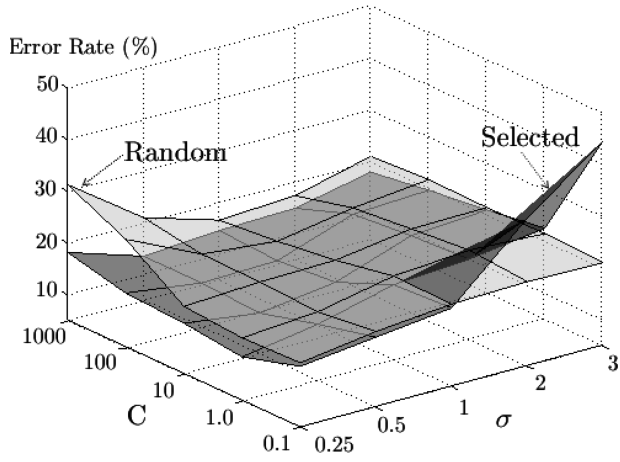
sensitive to hyperparameter variation because the patterns are distributed all over the region. However, note that RAN never performs as well as ALL since random sampling inevitably misses many patterns of importance to SVM training. See the best result of RAN in Table 3. Figure 10 shows similar results for the sine function problem.

Table 3 summarizes the best results of ALL, SEL, and RAN for both problems. First, compared with the training time of ALL, that of SEL is little more than trivial because of the reduced size of training set. For both artificial problems, a standard QP solver, Gunn's SVM MATLAB toolbox, was used. Considering that model selection always involves multiple trials, an individual's reduction in training time can amount to a huge savings of time. Second, compared with RAN, SEL achieved an accuracy on a similar level to the best model of ALL while RAN could not. To show that there was no significant difference between ALL and SEL, we conducted the McNemar's test (Dietterich, 1998). The p-values between ALL and RAN, and also between ALL and SEL, are presented in the last row of Table 3. In principle, the McNemar's test determines whether classifier A is better than classifier B. A p-value of zero indicates a significant difference between A and B, and a value of one indicates no significant difference. Although the p-value between ALL and RAN is not less than 5% in each problem, one can still compare its degree of difference from the p-value between ALL and SEL in statistical terms.

Figure 11 visualizes the experimental results of Table 3 on both problems. The subfigures, 11.1 to 11.3, indicate the results of ALL, RAN, and SEL in order. The decision boundary is depicted as a solid line and the margin as a dotted line. Support vectors are outlined. The decision boundary of ALL



a. SEL VS. ALL

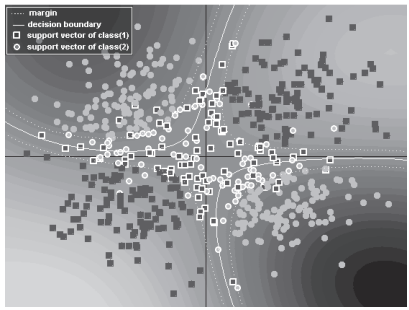


b. SEL VS. RAN

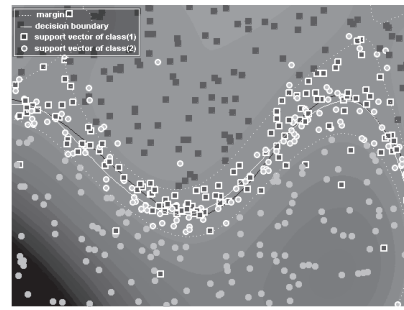
Figure 10: Performance comparison over hyperparameter variation: sine function problem.

looks more alike to that of SEL than to that of RAN. That explains why SEL produced similar results to ALL.

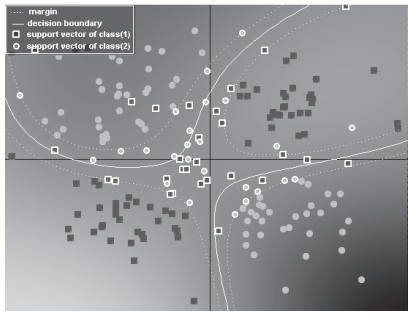
5.2 Benchmarking Data Sets. Table 4 presents the summary of the comparison results on various real-world benchmarking data sets (MNIST,



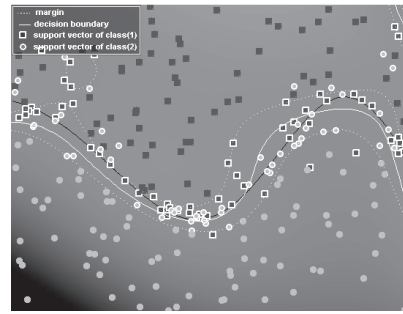
1.a. Continuous XOR: ALL



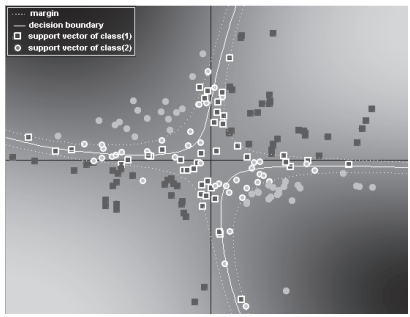
1.b. Sine Function: ALL



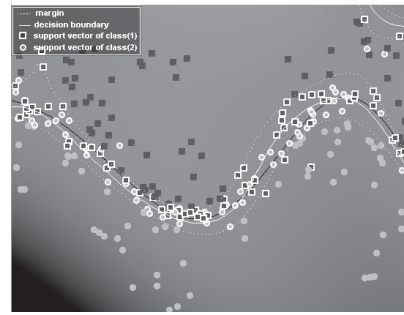
2.a. Continuous XOR: RAN



2.b. Sine Function: RAN



3.a. Continuous XOR: SEL



3.b. Sine Function: SEL

Figure 11: Patterns and SVM decision boundaries. A decision boundary is depicted as a solid line and the margins as the dotted lines. Support vectors are outlined. The decision boundary of ALL looks more alike to that of SEL than to that of RAN. This explains why SEL performed similar to ALL.

Table 4: Empirical Result for Benchmarking Data Sets.

		Number of Training Patterns	Number of Support Vectors	Preprocessing Time (Ratio)	Training Time (Ratio)	Test Error Rate (%)	McNemar's p-value
Continuous XOR: 1000 test patterns							
ALL	$C = 10, \sigma = 0.5$	600	167	–	1.00	**9.67**	–
RAN	$C = 100, \sigma = 1$	180	68	–	0.10	12.33	0.08
SEL	$C = 100, \sigma = 0.25, k = 5$	180	84	0.20	0.12	**9.67**	**1.00**
SVM-KM	$C = 1, \sigma = 0.25, k = 60$	308	149	0.78	0.16	10.00	0.69
Sine function: 1000 test patterns							
ALL	$C = 10, \sigma = 0.50$	500	250	–	1.00	**13.33**	–
RAN	$C = 0.1, \sigma = 0.25$	264	129	–	0.31	16.34	0.12
SEL	$C = 10, \sigma = 0.5, k = 5$	264	136	0.26	0.29	**12.67**	**0.89**
SVM-KM	$C = 50, \sigma = 0.25, k = 50$	335	237	2.04	0.27	14.00	0.81
4×4 Checkerboard: 10,000 test patterns							
ALL	$C = 20, \sigma = 0.25$	1000	172	–	1.00	**4.03**	–
RAN	$C = 50, \sigma = 0.5$	275	75	–	0.42	8.44	0.00
SEL	$C = 50, \sigma = 0.25, k = 4$	275	148	0.08	0.40	**4.66**	**0.76**
SVM-KM	$C = 20, \sigma = 0.25, k = 100$	492	159	49.13	0.33	5.20	0.00
Pima Indian Diabetes: 153 test patterns (5-cv out of 768 patterns)							
ALL	$C = 100, p = 2$	615	330	–	1.00	**29.90**	–
RAN	$C = 1, p = 1$	311	175	–	0.47	31.11	0.61
SEL	$C = 100, p = 2, k = 4$	311	216	0.13	0.58	30.30	**0.87**
SVM-KM	$C = 100, p = 2, k = 62$	561	352	0.48	0.98	**28.75**	0.72

Wisconsin Breast Cancer: 136 test patterns (5-cv out of 683 patterns)							
ALL	$C = 5, p = 3$	546	87	–	1.00	**6.80**	–
RAN	$C = 1, p = 1$	96	27	–	0.05	12.33	0.60
SEL	$C = 10, p = 3, k = 6$	96	41	0.01	0.06	**6.70**	**0.94**
SVM-KM	$C = 10, p = 3, k = 55$	418	85	17.08	0.62	11.02	0.53
MNIST: 3–8: 1984 test patterns							
ALL	$C = 10, p = 5$	11982	1253	–	1.00	**0.50**	–
RAN	$C = 10, p = 5$	4089	1024	–	0.15	0.86	0.19
SEL	$C = 50, p = 5, k = 50$	4089	1024	0.21	0.10	**0.45**	**0.42**
SVM-KM	$k = 1198$	NA	NA	NA	NA	NA	NA
MNIST: 6–8: 1932 test patterns							
ALL	$C = 10, p = 5$	11769	594	–	1.00	**0.25**	–
RAN	$C = 10, p = 5$	1135	185	–	0.03	0.83	0.01
SEL	$C = 20, p = 5, k = 50$	1135	421	0.20	0.07	**0.25**	**0.67**
SVM-KM	$k = 1177$	NA	NA	NA	NA	NA	NA
MNIST: 9–8: 1983 test patterns							
ALL	$C = 10, p = 5$	11800	823	–	1.00	**0.41**	–
RAN	$C = 10, p = 5$	1997	323	–	0.07	0.99	0.01
SEL	$C = 10, p = 5, k = 40$	1997	631	0.19	0.09	**0.43**	**0.57**
SVM-KM	$k = 1180$	NA	NA	NA	NA	NA	NA

1998; UCI, 1995), including the artificial data sets in the previous section. Again, SEL is compared with ALL and RAN, and another method is added as a competitor, SVM-KM (Almeida et al., 2000), which is a preprocessing method that reduces the training set based on k-means clustering algorithm.

The hyperparameters of SVM were chosen based on the best results using validation: C, σ, and p, indicate the misclassification tolerance, the width of RBF kernel, and the order of polynomial kernel, respectively. The parameter of SEL (NPPS), the number of neighbors k, was determined by the procedure in section 4 and appendix B (see also Shin & Cho, 2003b). And the parameter of SVM-KM, the number of clusters k, was set to 10% of the number of training patterns as recommended in Almeida et al. (2000). For the MNIST (1988) data set, we chose three binary classification problems; they are known as most difficult due to the similar shapes of the digits, for instance, the digit 3 looks similar to the digit 8. Most of the experiments were run on Pentium 4 with 1.9 GHz 512 RAM, whereas Pentium 4 with 3.0 GHz 1024 RAM for the MNIST problems. A standard QP solver lacks adequate memory capacity to handle the real-world data sets, so we chose an iterative SVM solver, OSU SVM Classifier Toolbox (Kernel Machines Organization, n.d.), after brief comparison about scalability with another candidate RSVM (Lee & Mangasarian, 2001). (Refer to appendix C for a comparison of the OSU SVM Classifier with RSVM.)

In Table 4, N/A denotes results that are not available. For ease of comparison, the computational time, preprocessing or SVM training, is shown as a ratio to the SVM training time of ALL. The best two results are represented as boldface in the test error rate. Similarly, the statistically most similar result with ALL is represented in boldface type in McNemar's p-value. The results show that the preprocessing by either SEL or SVM-KM is of great benefit to SVM training in reducing the training time. Particularly, if multiple runnings of SVM are required, one can take the benefit as many times as required. However, SVM-KM took longer than SEL, and, worse, it ran out of memory in large-sized problems. Also note that the pairwise test shows that SEL is more similar to ALL than any other method.

5.3 Real-World Marketing Data Set. The proposed algorithm was also applied to a marketing data set from (the Direct Marketing Association, n.d.). The data set DMEF4 has been used in other research (Ha, Cho, & MacLachlan, 2005; Malthouse, 2001, 2002). It is concerned with an upscale gift business that mails general or specialized catalogs to customers. The task predicts a customer will respond to the offering during the test period, September 1992 to December 1992. A customer who received the catalog and buys the product is labeled $+1$; otherwise, he or she is labeled -1. The training set is given based on the period December 1971 to June 1992. There are 101,532 patterns in the data set, each representing the purchase history information of a customer. We derived 17 input variables out of 91 original ones just as in Ha et al. (2005) and Malthouse (2001).

To show the effectiveness of SEL, we compared it with seven RANs because random sampling has most commonly been employed when researchers in this field attempt to reduce the size of the training set. Table 5 shows the models: RAN* denotes an SVM trained with random samples, where $*$ indicates the ratio of random samples drawn without replacement. Each model was trained and evaluated by using five-fold cross-validation. The hyperparameters of SVM were determined from $(C, \sigma) = \{0.1, 1, 10, 100, 1000\} \times \{0.25, 0.5, 1, 2, 3\}$. The number of neighbors (k) for SEL was set to 4. The OSU SVM Classifier was used as an SVM solver (Kernel Machines Organization, n.d.). Typically, a DMEF data set (Direct Marketing Association, n.d.) has a severe class imbalance problem because the response rate for the retailer's offer is very low: 9.4% for DMEF4. In that case, an ordinary accuracy measure tends to mislead us about the results by giving more weight to the heavily represented class. Thus, we used another accuracy measure, Balanced Correct-classification Rate (BCR), defined as

$$\text{Balanced Correct-classification Rate (BCR)} = \left(\frac{m_{11}}{m_1}\right) \cdot \left(\frac{m_{22}}{m_2}\right),$$

where m_i denotes the size of class i and m_{ii} is the number of patterns correctly classified into class i. Now the performance measure is balanced between two different class sizes.

Figure 12 shows the BCRs of the eight SVM models, and Table 6 presents the details. More patterns result in higher BCR among RAN*'s. However, the training time also increases proportionally to the number of training patterns, with the peak of 4820 sec for RAN100. SEL takes only 68 sec, and 129 sec if the NPPS running time is included. Note that one should perform SVM training several times to find a set of optimal hyperparameters, but only once for NPPS ahead of the whole procedure of training. In the last column of the table, the p-value of McNemar's test is listed when SEL is compared with an individual RAN*. There is a statistically significant difference between SEL and RAN up to RAN60 in accuracy, but no difference between SEL and RAN80 or RAN100. Overall, SEL achieves almost the same accuracy as RAN80 or RAN100 only with the number of training patterns comparable to RAN10 or RAN20.

6 Conclusions and Discussion

In this letter, we introduced an informative sampling method for the SVM classification task. By preselecting the patterns near the decision boundary, one can relieve the computational burden during SVM training. In the experiments, we compared the performance of the selected pattern set (SEL) by NPPS with that of a random sample set (RAN) and that of the original training set (ALL). We also compared the proposed method with a

Table 5: SVM Models.

Model (C, σ)	RAN05 (100, 1)	RAN10 (100, 1)	RAN20 (100, 0.5)	RAN40 (100, 0.5)	RAN60 (10, 1)	RAN80 (10, 0.5)	RAN100 (10, 0.5)	SEL (10, 0.5)
Number of patterns	4060 (5%)	8121 (10%)	16,244 (20%)	32,490 (40%)	48,734 (60%)	64,980 (80%)	81,226 (100%)	8871, Average

Notes: RAN* denotes an SVM trained with random samples, where $*$ indicates the percentage of random sampling. Note that RAN100 corresponds to ALL. The number of patterns of SEL slightly varies with the given set of each fold of 5-CV, and thus, it is represented as an average.

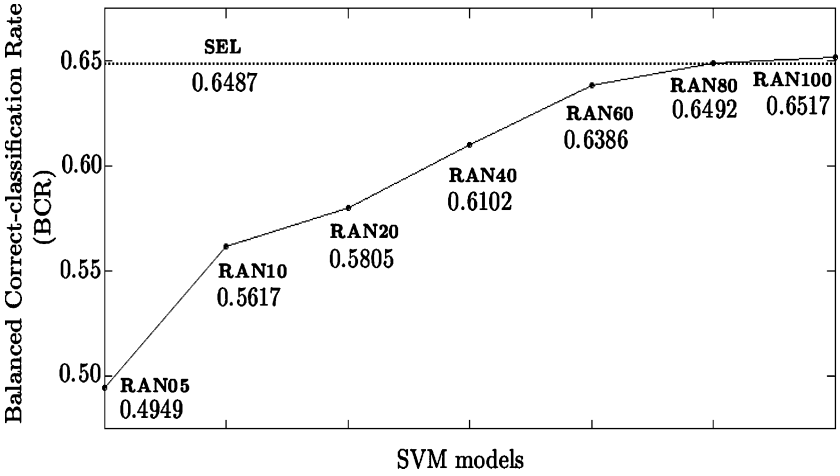


Figure 12: Balanced Correct-classification Rate (BCR): RAN* is depicted as a filled circle, and SEL is represented as a dotted reference line.

Table 6: Empirical Result for a Real-World Marketing Data Set, DMEF4

	Number of Training Patterns	Number of Support Vectors	Training Time (sec)	Correct Rate, BCR (%)	McNemar's Test (p-value)
RAN05	4060	1975	13.72	49.49	0.00
RAN10	8121	4194	56.67	56.17	0.00
RAN20	16,244	7463	149.42	58.05	0.00
RAN40	32,490	14,967	652.11	61.02	0.04
RAN60	48,734	22,193	1622.06	63.86	0.08
RAN80	64,980	28,968	2906.97	64.92	0.64
RAN100	81,226	35,529	4820.06	65.17	0.87
SEL	8871	6624	68.29	64.92	–

competing method, SVM-KM (Almeida et al., 2000). Through the comparison of synthetic and real-world problems, we empirically validated the efficiency of the proposed algorithm. SEL achieved an accuracy similar to that of ALL, while the computational cost was still similar to that of RAN with 10% or 20% of the samples. When compared with SVM-KM, SEL achieved better computational efficiency.

Here, we would like to address some future work. First, SVM solves a multiclass problem by a divide-and-combine strategy, which divides the multiclass problem into several binary subproblems (e.g., one-versus-others or one-versus-one) and then combines the outputs. This has led to the application of NPPS to binary class problems. However, NPPS can readily be extended to multiclass problems without major correction. Second, NPPS

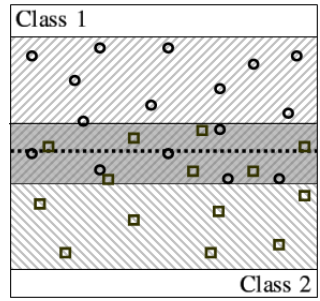
can also be utilized to reduce the lengthy training time of neural network classifiers. But it is necessary to add extra correct patterns to the selected pattern set to enhance the overlap region near the decision boundary (Choi, & Rockett, 2002; Hara & Nakayama, 2000). The rationale is that overlap patterns located on the "wrong" side of the decision boundary would lengthen the MLP training time. The derivatives of the backpropagated errors will be very small when evaluated at those patterns since they are grouped in a narrow region on either side of the decision boundary. By adding extra correct patterns, however, the network training will converge faster. In the meantime, the idea of adding some randomly selected patterns to SEL may also relieve the higher sensitivity of SEL to hyperparameter variation (see Figure 9). If the high sensitivity is caused by "narrow" distribution of the selected patterns, it can be relaxed by some random patterns from "overall" input space. But the mixing ratio of the patterns from SEL and from RAN requires further study. Third, the current version of NPPS works for classification problems only, and thus is not applicable to regression problems. A straightforward idea for regression would be to use the mean (μ) and variance (Σ) of k nearest neighbors' outputs. A pattern having a small value of Σ can be replaced by μ of its neighbors, including itself. That is, $k+1$ patterns can be replaced by one pattern. On the contrary, a pattern having a large value of Σ can be totally eliminated since in a regression problem, the patterns located away from major group, such as outliers, are less important to learning. But its neighbors should be used to explore the next pattern. Similar research based on ensemble neural network was conducted by Shin and Cho (2001). Fourth, one of interesting future directions is the effort to extend NPPS for data with concept drift (Aha, Kibler, & Albert, 1991; Bartlett, Ben-David, & Kulkarni, 2000; Helmbold & Long, 1994; Klinkenberg, 2004; Pratt & Tschapek, 2003; Stanley, 2003; Widmer & Kubat, 1996). In concept drift, the decision boundary changes as data arrive in the form of a stream. A naive approach would be to employ a moving window over the data stream and then run NPPS repeatedly. For better results, NPPS should be substantially modified and rigorously tested.

Appendix A: Empirical Complexity Analysis

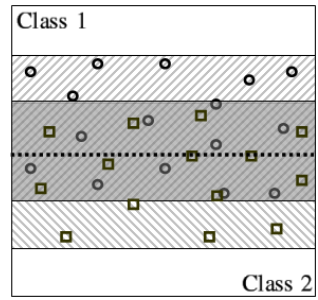
We empirically show that NPPS runs in approximately vM, where M is the number of training patterns and v is the number of overlap patterns (a full theoretical analysis is available in Shin & Cho, 2003a). A total of M patterns, half from each class, were randomly generated from a pair of two-dimensional uniform distributions:

$$C_1 = \left\{ \vec{x} \mid U\left(\begin{bmatrix} -1 \\ (0 - \frac{1}{2}\frac{v}{M}) \end{bmatrix} < \vec{x} < \begin{bmatrix} 1 \\ (1 - \frac{1}{2}\frac{v}{M}) \end{bmatrix} \right) \right\},$$

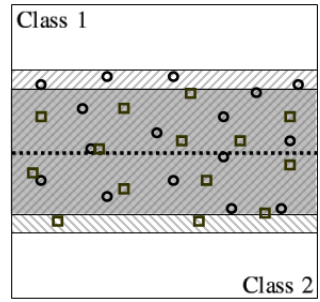
$$C_2 = \left\{ \vec{x} \mid U\left(\begin{bmatrix} -1 \\ (-1 + \frac{1}{2}\frac{v}{M}) \end{bmatrix} < \vec{x} < \begin{bmatrix} 1 \\ (0 + \frac{1}{2}\frac{v}{M}) \end{bmatrix} \right) \right\}.$$



a. $v = 0.3M$



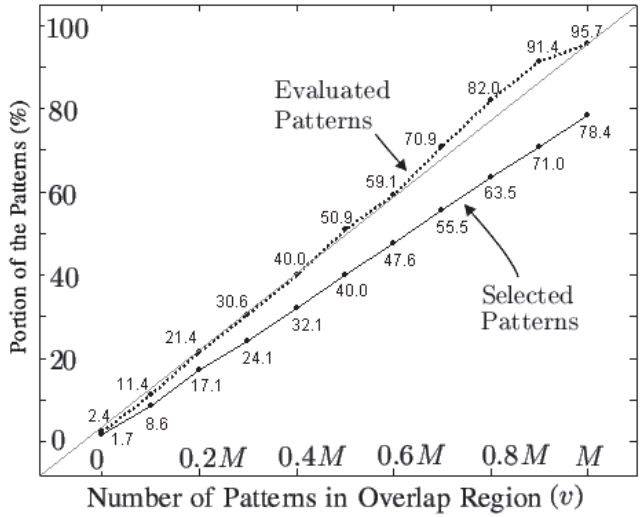
b. $v = 0.5M$



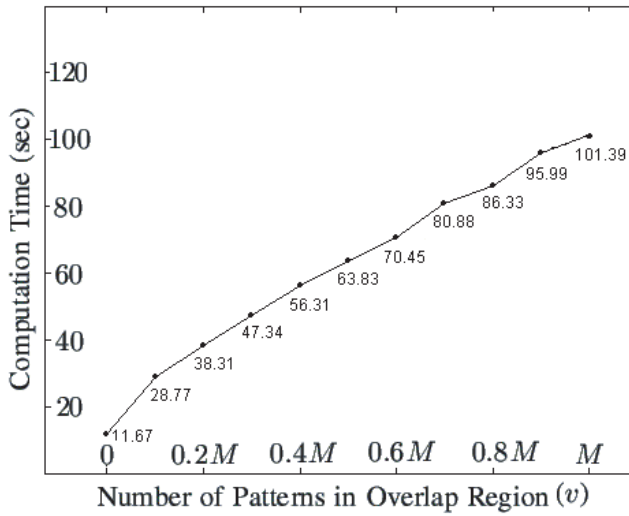
c. $v = 0.7M$

Figure 13: Overlap of two uniform distributions. The dark gray area is the overlap region that contains v patterns. The number of overlap patterns, v, is set to every decile of training set size, M. (a, b, c) $v = 0.3M$, $v = 0.5M$, and $v = 0.7M$, respectively.

We set v to every decile of M : $v = 0, 0.1M, 0.2M, \ldots, 0.9M, M$. Figure 13 shows the distributions of $v = 0.3M$, $v = 0.5M$, and $v = 0.7M$. The larger values of v correspond to more overlap patterns. We set out to see how the computation time of NPPS works with the changing value of v—in particular, whether the computation time is linearly proportional to v as

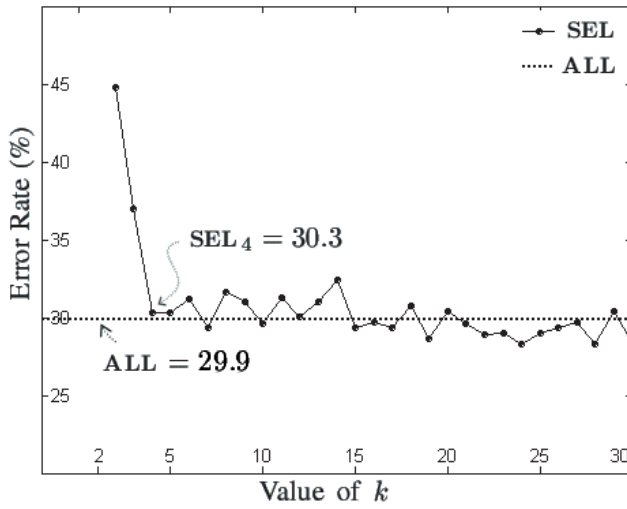


a. The number of selected patterns (%)

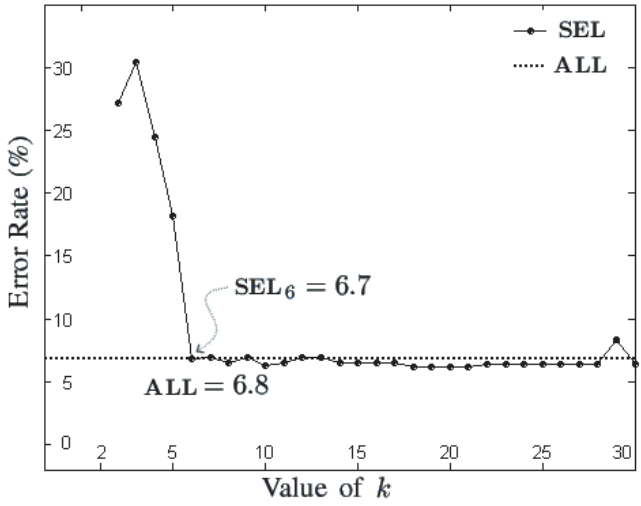


b. Computation time

Figure 14: Empirical complexity analysis: NPPS with increasing number of overlap patterns v.



a. Pima Indians Diabetes ($k^* = 4$)



b. Wisconsin Breast Cancer ($k^* = 6$)

Figure 15: SVM test error rates. The error rate is stabilized at about 30.0% for Pima Indian Diabetes when $k \geq 4$ and at about 6.7% for Wisconsin Breast Cancer when $k \geq 6$.

Table 7: Empirical Comparison on Different SVM Solvers.

		Number of Training Patterns	Time Ratio: Training	Test Error Rate (%)	McNemar's p-Value
Continuous XOR: 1000 test patterns					
OSU-SVM	$C = 10, \sigma = 0.5$	600	1.00	9.67	–
RSVM	$C = 10, \sigma = 0.5$	600	1.20	9.97	0.79
Sine function: 1000 test patterns					
OSU-SVM	$C = 10, \sigma = 0.50$	500	1.00	13.33	–
RSVM	$C = 100, \sigma = 0.25$	500	0.31	13.46	0.85
4×4 checkerboard: 10,000 test patterns					
OSU-SVM	$C = 20, \sigma = 0.25$	1000	1.00	4.03	–
RSVM	$C = 100, \sigma = 0.25$	1000	1.87	3.88	0.00
Pima Indian Diabetes: 153 test patterns (5-cv out of 768 patterns)					
OSU-SVM	$C = 100, p = 2$	615	1.00	29.90	–
RSVM	$C = 10, p = 1$	615	0.10	29.64	0.72
Wisconsin Breast Cancer: 136 test patterns (5-cv out of 683 patterns)					
OSU-SVM	$C = 5, p = 3$	546	1.00	6.80	–
RSVM	$C = 10, p = 3$	546	1.65	8.02	0.45
MNIST: 3–8: 1984 test patterns					
OSU-SVM	$C = 10, p = 5$	11982	1.00	0.50	–
RSVM		11982	N/A	N/A	N/A
MNIST: 6–8: 1932 test patterns					
OSU-SVM	$C = 10, p = 5$	11769	1.00	0.25	–
RSVM		11769	N/A	N/A	N/A
MNIST: 9–8: 1983 test patterns					
OSU-SVM	$C = 10, p = 5$	11800	1.00	0.41	–
RSVM		11800	N/A	N/A	N/A

mentioned. Figure 14a shows the number of selected patterns through evaluation when v grows from 0 up to $M = 10,000$. In Figure 14b, one can clearly see that the computation time is proportional to v.

Appendix B: Experiments on the Number of Neighbors

Based on the procedure presented in Figure 7, we briefly present experiments on Pima Indian Diabetes and Wisconsin Breast Cancer. According to the procedure, the lower bounds of v were estimated as 393 and 108 from the training error rates, $P_{error} = 32.0\%$ and $P_{error} = 9.9\%$, respectively. These led to $k^* = 4$ in Pima Indian Diabetes and $k^* = 6$ in Wisconsin Breast Cancer. (The values of $k^{\min}$ were also 4 and 6, respectively.) Figure 15

shows that the test error rate stabilizes at about 30.0% for Pima Indian Diabetes when $k \geq 4$, and at about 6.7% for Wisconsin Breast Cancer when $k \geq 6$.

Appendix C: Empirical Comparison on SVM Solvers

We provide a short comparison between OSU-SVM (OSU SVM Classifier, Kernel Machines Organization) and RSVM (Lee & Mangasarian, 2001), which are known as the fastest SVM learning algorithms. All of the experimental settings were as identified in section 5.2. The parameter of RSVM, the random sampling ratio, was set to 5% to 10% of training patterns according to Lee and Mangasarian. In Table 7, the computational time of RSVM is shown as a ratio to the SVM training time of OSU-SVM. The results show that both of the algorithms are almost similar in accuracy. Also in training time, it is hard to tell which is superior to the other. However, RSVM was not available for the MNIST (1998) problems. It failed to load the kernel matrix on the memory (note that RSVM is not an iterative solver). Therefore, we chose to use OSU-SVM as a base learner in our experiment because it is relatively more scalable and also parameter free.

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