Classification by Set Cover: The Prototype Vector Machine

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Abstract

We introduce a new nearest-prototype classifier, the prototype vector machine (PVM). It arises from a combinatorial optimization problem which we cast as a variant of the set cover problem. We propose two algorithms for approximating its solution. The PVM selects a relatively small number of representative points which can then be used for classification. It contains 1-NN as a special case. The method is compatible with any dissimilarity measure, making it amenable to situations in which the data are not embedded in an underlying feature space or in which using a non-Euclidean metric is desirable. Indeed, we demonstrate on the much studied ZIP code data how the PVM can reap the benefits of a problem-specific metric. In this example, the PVM outperforms the highly successful 1-NN with tangent distance, and does so retaining fewer than half of the data points. This example highlights the strengths of the PVM in yielding a low-error, highly interpretable model. Additionally, we apply the PVM to a protein classification problem in which a kernel-based distance is used.

1 Introduction

Suppose we are given a set of training points $X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^p$ with corresponding class labels $y_1, \ldots, y_n \in \{1, \ldots, L\}$ and, in addition, a set of unlabeled points $Z = \{z_1, \ldots, z_m\} \subset \mathbb{R}^p$. Our goal is to choose a relatively small set of prototypes $P_l \subseteq Z$ for each class $l$ in such a way that the

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collection $\mathcal{P}_1, \ldots, \mathcal{P}_L$ represents a summary or distillation of the training set (i.e., someone given only $\mathcal{P}_1, \ldots, \mathcal{P}_L$ would have a good sense of the original training data, $\mathcal{X}$ and $y$). While our default choice is $\mathcal{Z} = \mathcal{X}$, we find it notationally easier to differentiate between the two sets. When $\mathcal{Z} = \mathcal{X}$, we are in the standard setting of a condensation problem [Ripley, 2005].

Having a well-selected set of prototypes $\mathcal{P}_1, \ldots, \mathcal{P}_L \subseteq \mathcal{Z}$ is advantageous for two main reasons: interpretability and classification. For domain specialists, examining a handful of representative examples of each class can be highly informative especially when $n$ is large (since looking through all examples from the original data set could be overwhelming or even infeasible). Intuitively, a well-chosen set $\mathcal{P}_l \subseteq \mathcal{Z}$ of prototypes for class $l$ should capture the full spread of variation within this class while also taking into account how class $l$ differs from other classes. Finally, the relative number of prototypes in each class should be determined by the complexity of that class.

The other major use of the prototypes is for classification. Once we have prototype sets $\mathcal{P}_1, \ldots, \mathcal{P}_L$, we may classify any new $x \in \mathbb{R}^p$ according to the class whose $\mathcal{P}_l$ contains the nearest prototype:

$$\hat{c}(x) = \arg\min_{l} \min_{z \in \mathcal{P}_l} d(x, z).$$

(1)

Notice that this classification rule reduces to 1-nearest-neighbors (1-NN) in the case that $\mathcal{P}_l$ consists of all $x_i \in \mathcal{X}$ with $y_i = l$.

In this paper, we introduce the prototype vector machine (PVM), which describes a particular choice for the sets $\mathcal{P}_1, \ldots, \mathcal{P}_L$. At its heart is the premise that $\mathcal{P}_l$ should consist of points that are close to many training points of class $l$ and are far from training points of other classes. This intuition captures the sense in which the word “prototypical” is commonly used.

In Section 2 we begin with a conceptually simple optimization criterion that describes a desirable choice for $\mathcal{P}_1, \ldots, \mathcal{P}_L$. We express this idea as an integer program and then in Section 3 present two approximation algorithms for it. Section 4 discusses considerations for applying the PVM most effectively to a given data set. In Section 5 we give an overview of related work. In Section 6 we demonstrate the PVM’s effectiveness—both in terms of classification accuracy and ease of interpretation—on a number of real data sets, including the much-studied ZIP code digits data set.

Finally, a note on the name: The PVM has a number of similarities with the Support Vector Machine: sparsity in the samples and the slack
formulation. The PVM integer program is an extension of the set cover problem, which we review presently.

1.1 The set cover integer program

Consider the two sets $\mathcal{X}$ and $\mathcal{Z}$ but without the labels $y$. Let $D$ be the $n \times m$ matrix of dissimilarities, with $D_{ij} = d(x_i, z_j)$ for each $x_i \in \mathcal{X}$ and $z_j \in \mathcal{Z}$ (note: $d$ need not be a metric), and fix $\epsilon > 0$. The goal is to find the smallest subset of points $\mathcal{P} \subseteq \mathcal{Z}$ such that every point $x_i \in \mathcal{X}$ is within $\epsilon$ of some point in $\mathcal{P}$ (i.e., there exists $z_j \in \mathcal{P}$ with $d(x_i, z_j) < \epsilon$). Let $B_\epsilon(x) = \{x' \in \mathbb{R}^p : d(x', x) < \epsilon\}$ denote the ball of radius $\epsilon$ centered at $x$.

Introducing the indicator variables

$$
\alpha_j = \begin{cases} 
1 & \text{if } z_j \in \mathcal{P} \\
0 & \text{otherwise,} 
\end{cases}
$$

this problem can be stated as an integer program:

$$
\text{minimize} \quad \sum_{j=1}^{m} \alpha_j \\
\text{subject to} \quad \sum_{j : x_i \in B_\epsilon(z_j)} \alpha_j \geq 1 \quad \forall x_i \in \mathcal{X} \\
\alpha_j \in \{0, 1\} \quad \forall z_j \in \mathcal{Z}.
$$

The objective is simply $|\mathcal{P}|$. The summation in the constraint counts the number of elements of $\mathcal{P}$ that are within $\epsilon$ of the point $x_i$, so a feasible solution to the above integer program is one that has at least one prototype within $\epsilon$ of each training point.

From a machine learning point of view, set cover can be seen as a clustering problem in which we wish to find the smallest number of clusters such that every point is within $\epsilon$ of at least one cluster center. In the language of vector quantization, it seeks the smallest codebook (restricted to $\mathcal{Z}$) such that no vector is distorted by more than $\epsilon$ [Tipping and Schölkopf 2001].

2 The prototype vector machine

The prototype vector machine is an extension of the set cover problem to the supervised learning context (in which each $x_i \in \mathcal{X}$ has a class label $y_i$). The PVM seeks a set of prototypes for each class that is optimal in a sense
Figure 1: Given a value for $\epsilon$, the choice of $P_1, \ldots, P_L$ induces $L$ partial covers of the training points by $\epsilon$-balls centered at each prototype. Here $\epsilon$ is varied from the smallest interpoint distance (upper-left) to approximately the median interpoint distance (lower-right).

that will be made precise in what follows. For a given choice of $P_l \subseteq Z$, we consider the set of $\epsilon$-balls centered at each $z_j \in P_l$ (see Figure 1). A desirable prototype set for class $l$ is one that induces a set of balls which
(a) covers as many training points of class $l$ as possible,
(b) covers as few training points as possible of classes other than $l$,
and (c) is sparse (i.e., uses as few prototypes as possible for the given $\epsilon$).

2.1 PVM as an integer program

We now express the three properties above as an integer program, taking as a starting point the set cover problem of Equation 2. Property (b) suggests that in certain cases it may be necessary to leave some points of class $l$ uncovered. For this reason, we adopt a prize-collecting set cover framework for our problem (i.e., we assign a cost to each covering set, a penalty for being uncovered to each point, and then find the minimum-cost partial cover, Könenmann et al. 2006). Let $\alpha_j^{(l)} \in \{0, 1\}$ indicate whether we choose $z_j$ to be in $P_l$ (i.e., to be a prototype for class $l$). We define the PVM to be a
solution to the following integer program:

$$\begin{align*}
\text{minimize} & \quad \alpha_j^{(l)} \xi_i + \sum_i \eta_i + \lambda \sum_{j,l} \alpha_j^{(l)} \\
\text{subject to} & \quad \sum_{j:x_i \in B_i(x_j)} \alpha_j^{(y_i)} \geq 1 - \xi_i \quad \forall x_i \in \mathcal{X} \\
& \quad \sum_{j:x_i \in B_i(x_j)} \alpha_j^{(l)} \leq 0 + \eta_i \quad \forall x_i \in \mathcal{X} \\
& \quad \alpha_j^{(l)} \in \{0,1\} \quad \forall z_j \in \mathcal{Z}, l \in \{1,\ldots,L\} \\
& \quad \xi_i, \eta_i \geq 0 \quad \forall x_i \in \mathcal{X}
\end{align*}$$

We have introduced two slack variables, $\xi_i$ and $\eta_i$, per training point $x_i$. Constraint (3a) enforces that each training point be covered by at least one ball of its own class-type (otherwise $\xi_i = 1$). Constraint (3b) expresses the condition that training point $x_i$ not be covered with balls of other classes (otherwise $\eta_i > 0$). In particular, the slack variables can be interpreted as

- $\xi_i = \begin{cases} 1 & \text{if } x_i \text{ is not covered by a class-}y_i \text{ prototype ball} \\ 0 & \text{otherwise} \end{cases}$
- $\eta_i = \text{Number of prototypes covering } x_i \text{ that are not of class } y_i.$

Finally, $\lambda \geq 0$ is a parameter specifying the cost of adding a prototype. Its effect is to control the number of prototypes chosen (corresponding to property (c) of the last section). We generally choose $\lambda = 1/n$, so that property (c) serves only as a “tie-breaker” for choosing among multiple solutions that do equally well on properties (a) and (b). Hence, in words, we are minimizing the sum of (a) the number of points left uncovered, (b) the number of points wrongly covered, and (c) the number of covering balls (multiplied by $\lambda$). The resulting method has a single tuning parameter, $\epsilon$ (the ball radius), which can be estimated by cross validation.

We show in the Appendix that the PVM integer program is equivalent to $L$ separate prize-collecting set cover problems. Let $\mathcal{X}_l = \{ x_i \in \mathcal{X} : y_i = l \}$.
Then, for each class $l$, the set $P_l \subseteq Z$ is given by the solution to

$$\begin{align*}
&\text{minimize } \sum_{j=1}^{m} C_l(j) \alpha_l(j) + \sum_{x_i \in X_l} \xi_i \\
&\text{subject to } \sum_{j : x_i \in B_l(z_j)} \alpha_l(j) \geq 1 - \xi_i \quad \forall x_i \in X_l \\
&\quad \alpha_l(j) \in \{0, 1\} \quad \forall z_j \in Z \\
&\quad \xi_i \geq 0 \quad \forall x_i \in X_l
\end{align*}$$

where $C_l(j)$ is the cost of adding $z_j$ to $P_l$ and a unit penalty is charged for each point $x_i$ of class $l$ left uncovered. The cost of a covering set for the PVM is the number of miscovered points plus a baseline charge of $\lambda$:

$$C_l(j) = \lambda + |B_{\epsilon}(z_j) \cap (X \setminus X_l)|.$$ 

3 Solving the problem: two approaches

The prize-collecting set cover problem can be transformed to a standard set cover problem [Könemann et al., 2006], which is itself NP-hard, so we do not expect to find a polynomial-time algorithm to solve the general PVM problem exactly. Further, certain inapproximability results have been proven for the set cover problem [Feige, 1998]. In what follows, we present two algorithms for approximately solving our problem.

3.1 LP relaxation with randomized rounding

A well-known approach for the set cover problem is to relax the integer constraint $\alpha_l(j) \in \{0, 1\}$ by replacing it with $0 \leq \alpha_l(j) \leq 1$. The result is a linear program (LP), which is convex and easily solved with any LP solver. The result is subsequently rounded to recover a feasible (though not necessarily optimal) solution to the original integer program.

Let $\{\alpha^{*l}_j\}$ denote a solution to the LP. Since our solution in general will be fractional, we adopt the following rounding strategy to produce an integral solution: For each $j \in \{1, \ldots, m\}$ and $l \in \{1, \ldots, L\}$, we independently draw $A_l(j) \sim \text{Bernoulli}(\alpha^{*l}_j)$. Notice that $\alpha^{*l}_j \in [0, 1]$, so this approach is

\footnote{We do not assume in general that the dissimilarities satisfy the triangle inequality, so we consider arbitrary covering sets.}
well-defined. Let $S_i$ and $T_i$ denote the slack (corresponding to $\xi_i$ and $\eta_i$) incurred by the rounded solution $\{A_j^{(l)}\}$. These random variables are given by

$$S_i = \begin{cases} 1 & \text{if } x_i \text{ uncovered} \\ 0 & \text{otherwise} \end{cases} \iff \sum_{j: x_i \in B_i(z_j)} A_j^{(y_i)} = 0$$

$$T_i = \sum_{l \neq y_i, j: x_i \in B_i(z_j)} A_j^{(l)}.$$  

(4)

The randomized rounding algorithm is as follows (with $B$ typically in the hundreds):

For $b = 1, \ldots, B$:

1. Draw independently $A_j^{(l)}(b) \sim \text{Bernoulli}(\alpha^{* (l)}_j)$.
2. Find the corresponding $S_i(b)$, $T_i(b)$ making this a feasible solution.
3. Evaluate objective $OBJ(b) = \sum_{i=1}^n (S_i(b) + T_i(b)) + \lambda \sum_{j,l} A_j^{(l)}(b)$.

Return $\{A_j^{(l)}(b)\}$ with minimum $OBJ(b)$.

In the Appendix, we prove that the expected objective on any iteration satisfies

$$E \left[ \sum_{i=1}^n (S_i(b) + T_i(b)) + \lambda \sum_{j,l} A_j^{(l)}(b) \right] \leq \frac{n}{e} + OPT_{LP} \leq \frac{n}{e} + OPT_{IP}$$

where $OPT_{LP} = \sum_{i=1}^n (\xi^*_i + \eta^*_i) + \lambda \sum_{j=1}^n \sum_{l=1}^L \alpha_j^{* (l)}$ is the optimal value of the LP (which is a lower bound on the integer program’s optimal value).

One disadvantage of this approach is that it requires solving an LP, which can be relatively slow and memory-intensive for large data sets. The approach we describe next is much lighter-weight and is thus our preferred method.

### 3.2 A greedy approach

Another well-known approximation algorithm for the set cover problem is the greedy algorithm [Vazirani, 2001]. At each step, we add the prototype that has the least ratio of cost to number of points newly covered. However,
here we present a less standard greedy algorithm which has certain practical advantages over the standard greedy approach and does not in our experience do noticeably worse in minimizing the PVM objective. At each step we find the $z_j \in Z$ and class $l$ for which adding $z_j$ to $P_l$ most decreases the objective function. That is, we find the $(z_j, l)$ pair with the best tradeoff of covering previously uncovered training points of class $l$ while avoiding covering points of other classes. The incremental improvement of going from $(P_1, \ldots, P_L)$ to $(P_1, \ldots, P_{l-1}, P_l \cup \{z_j\}, P_{l+1}, \ldots, P_L)$ can be denoted by $\Delta \text{Obj}(z_j, l) = \Delta \xi(z_j, l) - \Delta \eta(z_j, l) - \lambda$ where

$$\Delta \xi(z_j, l) = \left| \mathcal{X}_l \cap \left( B_{\epsilon}(z_j) \setminus \bigcup_{z_j' \in P_l} B_{\epsilon}(z_j') \right) \right|$$

$$\Delta \eta(z_j, l) = \left| B_{\epsilon}(z_j) \cap (\mathcal{X} \setminus \mathcal{X}_l) \right|$$

The greedy algorithm is simply as follows:

1. Start with $P_l = \emptyset$ for each class $l$.
2. While $\Delta \text{Obj}(z^*, l^*) > 0$:
   - Find $(z^*, l^*) = \arg\max_{(z_j, l)} \Delta \text{Obj}(z_j, l)$.
   - Let $P_{l^*} := P_{l^*} \cup \{z^*\}$.

4 Problem-specific considerations

The PVM provides a considerable amount of flexibility that allows the user to tailor it to the particular problem at hand.

4.1 Dissimilarities

The PVM depends on all of the $x_i$ and $z_j$ only through the pairwise dissimilarities $d(x_i, z_j)$ and can accept any matrix with non-negative entries. This allows it to share in the benefits of kernel methods by using a kernel-based distance. Also, for problems in the $p \gg n$ realm, using distances that effec-

\[ d(x, x') = \sqrt{K(x, x) + K(x', x') - 2K(x, x')} \]

\[ 2 \text{Given a kernel } K(x, x'), \text{ we can use the distance} \]

\[ d(x, x') = \sqrt{K(x, x) + K(x', x') - 2K(x, x')} \]
tively lower the dimension can lead to improvements. For instance, we have achieved gains in classification accuracy in some \( p \gg n \) simulations by using the DANN-distance [Hastie and Tibshirani 1996], which is a supervised measure of distance. Additionally, in certain problems (e.g., in proteomics, see Section 6.3) the data may not be readily embedded in a vector space. In such a case, we may still apply the PVM if pairwise dissimilarities are available.

Finally, given any dissimilarity \( d \), we may instead use \( \tilde{d} \), defined by \( \tilde{d}(x, z) = |\{x_i \in \mathcal{X} : d(x_i, z) \leq d(x, z)\}| \). Using \( \tilde{d} \) induces \( \epsilon \)-balls \( B_\epsilon(z_j) \) containing the \( |\lfloor \epsilon \rfloor - 1 \) nearest training points to \( z_j \).

4.2 Prototypes not on training points

Another inherent flexibility of the PVM is in the choice of \( Z \), the set of potential prototypes. While \( Z = \mathcal{X} \) is a standard choice, we have experimented with other possibilities as well. For example, if we are also given a set of unlabeled data (e.g., a test set), we may add these examples as potential prototypes, yielding a semi-supervised version of the PVM. Doing so preserves the property that all prototypes are actual examples (rather than arbitrary points in \( \mathbb{R}^p \)).

We believe that having prototypes confined to lie on actual observed points is desirable for interpretability. However, in circumstances in which this property is not needed, \( Z \) may be further augmented to include other points. For example, one could run \( K \)-means on each class’s points individually (or on the training set as a whole) and add these \( L \cdot K \) centroids to \( Z \). This method seems to help especially in high dimensional problems where constraining all prototypes to lie on data points suffers from the curse of dimensionality. Another successful choice for \( Z \) is to sample uniformly within the convex hull of each class’s training points.

5 Related Work

Before presenting the PVM’s empirical performance on data sets, we discuss its relation to several pre-existing methods. The PVM with \( Z = \mathcal{X} \) selects a subset of the original training set as prototypes. In this sense, it is similar in spirit to condensing and data editing methods, such as the condensed nearest neighbor rule [Hart 1968] and multiedit [Devijver and Kittler 1982]. Hart [1968] introduces the notion of the minimal consistent subset—the smallest subset of \( \mathcal{X} \) for which nearest-prototype classification has 0 training error. The PVM objective, \( \sum_{i=1}^{n} \xi_i + \sum_{i=1}^{n} \eta_i + \lambda \sum_{j,l} \alpha_{jl}^{(l)} \),
represents a sort of compromise, governed by $\lambda$, between consistency (first two terms) and minimality (third term). In future work, we will investigate formulations similar to PVM more closely directed toward the goal of the minimal consistent subset.

In a similar vein, an interesting connection can be drawn to the recent work of [Weinberger and Saul 2009] in which they introduce large margin nearest neighbor classification (LMNN), a novel approach to learning a metric that is well-suited to $k$-NN. LMNN seeks a linear transformation of the feature space that brings same-class nearest neighbors closer together and makes opposing-class points farther apart with the goal of having each training point’s $k$ nearest neighborhood as homogenous (in class label) as possible. The motivating intuition is thus similar to that of the PVM, in particular properties (a) and (b) of Section 2. The obvious difference between the methods is in what they output: LMNN learns a metric whereas PVM selects prototypes.

Finally, we mention a few other nearest prototype methods. $K$-means and $K$-medoids are common unsupervised methods which produce prototypes. Simply running these methods on each class separately yields prototype sets $P_1, \ldots, P_L$. $K$-medoids is similar to PVM in that its prototypes are selected from a finite set. In contrast, $K$-means’s prototypes are not required to lie on training points, making the method adaptive. Probably the most widely used prototype method is learning vector quantization (LVQ, [Kohonen 2001]). It is an adaptive prototype method as well. Several versions of LVQ exist, varying in certain details, but each begins with an initial set of prototypes and then iteratively adjusts them in a fashion that tends to encourage each prototype to lie near many training points of its class and away from training points of other classes.

6 Examples on simulated and real data

We compare the PVM’s performance to some of the prototype methods mentioned above. For $K$-medoids, we run pam of the R package cluster on each class’s data separately, producing $K$ prototypes per class.

For LVQ, we use the functions lvqinit and olvq1 (optimized learning vector quantization 1, [Kohonen 2001]) from the R package class. We vary the initial codebook size to produce a range of solutions.
6.1 Mixture of Gaussians simulation

For demonstration purposes, we consider a three-class example with \( p = 2 \). Each class was generated as a mixture of 10 Gaussians (details given in the Appendix). Figure 1 shows the PVM solution for a range of values of the tuning parameter \( \epsilon \). In Figure 2, we display the classification boundaries for the PVM, \( K \)-medoids, and LVQ (taking the lowest test error solution for each method). Since we generated this example from a known model, we are able to compute the Bayes boundary. We see that the PVM succeeds in capturing the shape of the boundary. The erratic boundary of \( K \)-medoids highlights an advantage of the PVM over \( K \)-medoids; the latter does not consider the relation between classes when choosing prototypes and therefore does not perform well when classes overlap.

6.2 ZIP code digits data

We apply the PVM to the USPS handwritten digits data set which consists of a training set of \( n = 7291 \) grayscale (16 \( \times \) 16 pixel) images of handwritten digits 0-9 (and 2007 test images). We run the PVM for a range of values of \( \epsilon \) from the minimum interpoint distance (in which the PVM retains the entire training set and so reduces to 1-NN classification) to approximately the 14\(^{th}\) percentile of interpoint distances.

The lefthand panel of Figure 3 shows the test error as a function of the number of prototypes for several methods using the Euclidean metric. Since both LVQ and \( K \)-means can place prototypes anywhere in the feature space, which is advantageous in high-dimensional problems, we also allow PVM to select prototypes that do not lie on the training points by augmenting \( Z \). In this case, we run 10-means clustering on each class separately and then
The notion of the tangent distance between two such images was introduced by Simard et al. [1993] to account for certain invariances in this problem (e.g., the thickness and orientation of a digit are not relevant factors when we consider how similar two digits are). Use of tangent distance with 1-NN attained the lowest test errors of any method [Hastie and Simard, 1998]. Since the PVM operates on an arbitrary dissimilarities matrix, we can easily use the tangent distance in place of the standard Euclidean metric. The righthand panel of Figure 3 shows the test errors when tangent distance is used. $K$-medoids similarly readily accommodates any dissimilarity. While LVQ has been generalized to arbitrary differentiable metrics, there does not appear to be generic, off-the-shelf software available. The lowest test error attained by the PVM is 2.49% with a 3372-prototype solution (compared to 1-NN’s 3.09%). Also, we can see that for a wide range of $\epsilon$ values we get a solution with test error comparable to that of 1-NN, but requiring far fewer prototypes. An advantageous feature of the PVM is that it automatically chooses the number of prototypes per class to use. In this example, it is interesting to see the class-frequencies of prototypes (see Table 1).

The most dramatic feature of this solution is that it only retains seven of the 1005 examples of the digit 1. This reflects the fact that, relative to...
Table 1: Number of prototypes chosen per class

| Digit | 0  | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | Total |
|-------|----|----|----|----|----|----|----|----|----|----|-------|
| Training set | 1194 | 1005 | 731 | 658 | 652 | 556 | 664 | 645 | 542 | 644 | 7291 |
| PVM-best    | 493  | 7   | 661 | 551 | 324 | 486 | 217 | 101 | 378 | 154 | 3372 |

In this example, we took $Z = X$, so that each prototype is an actual handwritten digit from the training set (rather than being some linear combination of many handwritten digits). Figures 4 and 5 show images of the first 88 prototypes (of 3372) selected by the greedy algorithm. Above each image of Figure 4 is the number of training images previously uncovered that were correctly covered by the addition of this prototype and, in parentheses, the number of training points that are miscovered by this prototype. For example, we can see that the first prototype selected by the greedy algorithm, which was a “1,” covered 986 training images of 1’s and four training images that were not of 1’s. These four training images are shown in Figure 6. Indeed, all of them look very much like 1’s, which explains the algorithm’s confusion.

The lefthand panel of Figure 7 shows the improvement in the PVM objective, $\Delta \xi - \Delta \eta$, after each step of the greedy algorithm, revealing an
Figure 5: The first 88 prototypes (out of 3372) of the PVM-Greedy solution. We perform MDS (sammon, stress=0.07) on the tangent distances to visualize the prototypes in two dimensions.

Figure 6: The four training images that were miscovered by the first prototype of class 1 (see Figure 3).
interesting feature of the solution: we find that after the first 458 prototypes are added, each remaining prototype covers only one training point. Since in this example we took \( \mathcal{Z} = \mathcal{X} \) (and since a point always covers itself), this means that the final 2914 prototypes were chosen to cover only themselves. In this sense, we see that the PVM provides a sort of compromise between a sparse nearest prototype classifier and 1-NN. The compromise is determined by the prototype-cost parameter \( \lambda \). If \( \lambda > 1 \), the algorithm does not enter the 1-NN regime.

The righthand panel of Figure 7 shows the improvement in test error gained by running the greedy algorithm beyond the first 88 steps (corresponding to the \( \lambda = 6 \) solution). It is interesting to look at elements of the test set that are misclassified when we use just the 88 prototypes but are correctly classified when using the complete PVM-greedy solution (with all 3372 prototypes). There are 276 (out of 2007) such elements. Figure 8 shows a randomly chosen seven examples of these test points.

6.3 Protein Classification with String Kernels

In our next example, we present a case in which the patterns are not naturally represented as vectors in \( \mathbf{R}^p \). Leslie et al. [2004] study the problem of classification of proteins based on their amino acid sequences. They introduce a measure of similarity between protein sequences called the mismatch kernel. The general idea is that two sequences should be considered similar if they have a large number of short sequences in common (where two short sequences are considered the same if they have no more than a specified
Figure 8: Each row corresponds to a test digit that is misclassified using just the first 88 prototypes (which are shown in Figure 4). From left to right: the test digit itself, the nearest prototype among the 88 prototypes, the nearest prototype of the correct class (among the 88), and the nearest prototype in the full 3372-prototype solution. 

number of mismatches). We take as input a $1708 \times 1708$ matrix with $K_{ij}$ containing the value of the normalized mismatch kernel evaluated between proteins $i$ and $j$ (the data and software are from Leslie et al. 2004). The proteins fall into two classes, “Positive” and “Negative,” according to whether they belong to a certain protein family. We compute pairwise distances from this kernel via $D_{ij} = \sqrt{K_{ii} + K_{jj} - 2K_{ij}}$ and then run the PVM and K-medoids. Figure 9 shows the 10-fold cross-validated errors for the PVM and K-medoids. For the PVM, we take a range of equally-spaced quantiles of the pairwise distances from the minimum to the median for the parameter $\epsilon$. For K-medoids, we take as parameter the fraction of proteins in each class that should be prototypes. This choice of parameter allows the classes to have different numbers of prototypes, which is important in this example because the classes are greatly imbalanced (only 45 of the 1708 proteins are in class “Positive”). The minimum CV-error (1.76%) is attained by PVM using about 870 prototypes (averaged over the 10 models fit for that value of $\epsilon$). This error is identical to the minimum CV-error of a support vector machine (tuning the cost parameter) trained using this kernel. Fitting a model to the whole data set with the selected value of $\epsilon$, the PVM chooses 26 prototypes (of 45) for class “Positive” and 907 (of 1663) for class “Negative.”
Figure 9: Proteins data set. Recall that the rightmost point on the PVM curve corresponds to 1-NN classification.

6.4 UCI data sets

Finally, we run the PVM on six data sets from the UCI Machine Learning Repository [Asuncion and Newman, 2007] and compare its performance to that of 1-NN (i.e., retaining all training points as prototypes), K-medoids, and LVQ. We randomly select 2/3 of each data set for training and use the remainder as a test set. Ten-fold cross-validation (and the “1 standard error rule,” Hastie et al. [2009]) is performed on the training data to select a value for each method’s tuning parameter (except for 1-NN). Table 2 reports the error on the test set and the number of prototypes selected for each method. We see that in most cases PVM is able to do as well as or better than 1-NN but with a significant reduction in prototypes. No single method does best on all of the data sets.

7 Discussion

We have introduced a new prototype method, which can be used both for classification and for “summarizing” a data set. The PVM is the solution to a set cover problem which describes our notion of a desirable prototype set. Applying the PVM to the digits data highlights some of its strengths. First, it has competitive test error for a wide range of values of the tuning parameter. Its success in this example stems in part from its flexibility: it
Table 2: Test errors for the UCI data sets. For PVM, K-medoids, and LVQ, we used 10-fold cross validation (with the 1 SE rule) on the training set to tune the parameters.

| Data     | Test Error (%) | 1-NN | PVM | K-medoids | LVQ |
|----------|----------------|------|-----|-----------|-----|
| Diabetes | 28.9           | 24.2 | 33.2| 25.0      |     |
| Glass    | 38.0           | 36.6 | 39.4| 35.2      |     |
| Heart    | 21.1           | 21.1 | 17.8| 15.6      |     |
| Liver    | 41.7           | 41.7 | 40.0| 33.9      |     |
| Vowel    | 2.8            | 2.8  | 2.8 | 19.9      |     |
| Wine     | 3.4            | 11.9 | 6.8 | 3.4       |     |

was easily used with a problem-specific measure of dissimilarity. Additionally, it automatically chooses a suitable number of prototypes for each class. Particularly useful for interpretation is the fact that each PVM-prototype is an observation in the training set (i.e., is an actual hand drawn image). In medical applications, this would mean that prototypes correspond to actual patients. This feature may be of great practical use to domain experts for making sense of large data sets.

The PVM software will be made available as an R package in the R library.

8 Acknowledgements

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A PVM’s relation to prize-collecting set cover

Claim: Solving the PVM integer program is equivalent to solving $L$ prize-collecting set cover problems.

Proof. Recall that the PVM integer program is given by

\[
\begin{align*}
\text{minimize} & \quad \sum_{i=1}^{n} \xi_i + \sum_{i=1}^{n} \eta_i + \lambda \sum_{j,l} \alpha_{j}^{(l)} \\
\text{subject to} & \quad \sum_{j: \mathbf{x}_i \in B_r(\mathbf{z}_j)} \alpha_{j}^{(y_i)} \geq 1 - \xi_i \quad \forall \mathbf{x}_i \in \mathcal{X} \\
& \quad \sum_{j: \mathbf{x}_i \in B_r(\mathbf{z}_i) \land l \neq y_i} \alpha_{j}^{(l)} \leq 0 + \eta_i \quad \forall \mathbf{x}_i \in \mathcal{X} \\
& \quad \alpha_{j}^{(l)} \in \{0, 1\} \quad \forall \mathbf{z}_j \in \mathcal{Z}, l \in \{1, \ldots, L\} \\
& \quad \xi_i, \eta_i \geq 0 \quad \forall \mathbf{x}_i \in \mathcal{X}.
\end{align*}
\]

Now, the second set of inequality constraints is always tight, so we can
eliminate the slack variables \( \eta_1, \ldots, \eta_n \):

\[
\begin{align*}
\text{minimize} & \quad \sum_{i=1}^{n} \xi_i + \sum_{i=1}^{n} \sum_{j: x_i \in B_i(z_j), l \neq y_i} \alpha_j^{(l)} + \lambda \sum_{j,l} \alpha_j^{(l)} \\
\text{subject to} & \quad \sum_{j: x_i \in B_i(z_j)} \alpha_j^{(y_i)} \geq 1 - \xi_i \quad \forall x_i \in X \\
& \quad \alpha_j^{(l)} \in \{0, 1\} \quad \forall z_j \in \mathcal{Z}, l \in \{1, \ldots, L\} \\
& \quad \xi_i \geq 0 \quad \forall x_i \in X.
\end{align*}
\]

We can rewrite the second term of the objective as

\[
\begin{align*}
\sum_{i=1}^{n} \sum_{j: x_i \in B_i(z_j), l \neq y_i} \alpha_j^{(l)} & = \sum_{i=1}^{n} \sum_{j,l} 1\{x_i \in B_i(z_j), l \neq y_i\} \alpha_j^{(l)} \\
& = \sum_{j,l} \alpha_j^{(l)} \sum_{i=1}^{n} 1\{x_i \in D_j(\epsilon), x_i \notin X_l\} \\
& = \sum_{j,l} \alpha_j^{(l)} |B_k(z_j) \cap (X \setminus X_l)|
\end{align*}
\]

So the entire objective becomes

\[
\begin{align*}
\sum_{i=1}^{n} \xi_i + \sum_{j,l} \left[ (|B_k(z_j) \cap (X \setminus X_l)| + \lambda) \alpha_j^{(l)} \right]
\end{align*}
\]

Letting \( C_l(j) = \lambda + |B_k(z_j) \cap (X \setminus X_l)| \), the integer program may be written as

\[
\begin{align*}
\text{minimize} & \quad \sum_{l=1}^{L} \left[ \sum_{i \in X_l} \xi_i + \sum_{j=1}^{m} C_l(j) \alpha_j^{(l)} \right] \\
\text{subject to} & \quad \forall l \in \{1, \ldots, L\}, \\
& \quad \sum_{j: x_i \in B_i(z_j)} \alpha_j^{(l)} \geq 1 - \xi_i \quad \forall x_i \in X_l \\
& \quad \alpha_j^{(l)} \in \{0, 1\} \quad \forall z_j \in \mathcal{Z}, \forall l \in \{1, \ldots, L\} \\
& \quad \xi_i \geq 0 \quad \forall x_i \in X_l.
\end{align*}
\]
Written in this way, we see that both the objective and the constraints are separable with respect to class, meaning that the solution to the above is equivalent to solving $L$ integer programs (one for each $l \in \{1, \ldots, L\}$). The $l$th integer program has variables $\alpha^{(l)}_1, \ldots, \alpha^{(l)}_m$ and $\{\xi_i : x_i \in X_l\}$ and is given by

$$
\begin{align*}
&\text{minimize} \quad \sum_{j=1}^m C_l(j)\alpha^{(l)}_j + \sum_{x_i \in X_l} \xi_i \\
&\text{subject to} \quad \sum_{j : x_i \in B_{\epsilon}(z_j)} \alpha^{(l)}_j \geq 1 - \xi_i \quad \forall x_i \in X_l \\
&\quad \alpha^{(l)}_j \in \{0, 1\} \quad \forall z_j \in Z \\
&\quad \xi_i \geq 0 \quad \forall x_i \in X_l.
\end{align*}
$$

This is precisely the prize-collecting set cover problem (with unit penalty for leaving a point uncovered).

\[\square\]

## B Randomized Rounding Bound

**Claim:** Given the randomized rounding procedure described in Section 3.1, the objective on each iteration satisfies

$$E[OBJ] \leq \frac{n}{e} + OPT_{LP}.$$  

**Proof.** Let $\{\alpha^*_j, \xi^*_i, \eta^*_i\}$ denote a solution to the LP and recall that for each iteration, we sample independently

$$A^{(l)}_j \sim \text{Bernoulli}(\alpha^*_j).$$

The PVM objective on this iteration is given by

$$OBJ = \sum_{i=1}^n (S_i + T_i) + \lambda \sum_{j,l} A^{(l)}_j$$

where

$$S_i = \begin{cases} 
1 & \text{if } x_i \text{ uncovered} \iff \sum_{j : x_i \in B_{\epsilon}(z_j)} A^{(y_i)}_j = 0 \\
0 & \text{otherwise}
\end{cases}$$

$$T_i = \sum_{l \neq y_i} \sum_{j : x_i \in B_{\epsilon}(z_j)} A^{(l)}_j.$$
Now, by linearity of expectation, we have

\[
E[OBJ] = E \left[ \sum_{i=1}^{n} (S_i + T_i) + \lambda \sum_{j,l} A_j^{(l)} \right] = \sum_{i=1}^{n} (P(x_i \text{ uncovered}) + \eta_i^*) + \lambda \sum_{j,l} \alpha_j^{*(l)}
\]

since \( E[T_i] = \sum_{l \neq y_i} \sum_{j:x_i \in B_j(z_j)} \alpha_j^{*(l)} = \eta_i^* \).

Now,

\[
P(x_i \text{ uncovered}) = P \left( A_j^{(y_i)} = 0 \ \forall \ j : x_i \in B_j(z_j) \right) = \prod_{j:x_i \in B_j(z_j)} \left( 1 - \alpha_j^{*(y_i)} \right) \leq e^{-\sum_{j:x_i \in B_j(z_j)} \alpha_j^{*(y_i)}} \leq e^{-(1 - \xi_i^*)}
\]

using that \( 1-x \leq e^{-x} \) and, by LP feasibility (Constraint 3a), that \( -\sum_{j:x_i \in B_j(z_j)} \alpha_j^{*(y_i)} \leq -(1 - \xi_i^*) \). Now, \( 0 \leq \xi_i^* \leq 1 \) and

\[
e^x - 1 \leq \frac{1}{e} + \frac{e - 1}{e} x \quad \text{for} \quad 0 \leq x \leq 1
\]

so

\[
P(x_i \text{ uncovered}) \leq \frac{1}{e} + \frac{e - 1}{e} \xi_i^*
\]

from which it follows that

\[
E[OBJ] \leq \sum_{i=1}^{n} \left( \frac{1}{e} + \frac{e - 1}{e} \xi_i^* + \eta_i^* \right) + \lambda \sum_{j,l} \alpha_j^{*(l)} \leq \frac{n}{e} + \sum_{i=1}^{n} (\xi_i^* + \eta_i^*) + \lambda \sum_{j,l} \alpha_j^{*(l)} = \frac{n}{e} + OPT_{LP} \leq \frac{n}{e} + OPT_{IP}
\]

□
C Mixture of Gaussians example

We generate the data of Section 6.1 in the style of Hastie et al. [2009], Section 2.3.3. In particular,

- Fix 3 class centers $M_1, M_2, M_3 \in \mathbb{R}^2$, sampled from $N(0, 16I_2)$.
- For each class $k$, independently generate $m_1^{(k)}, \ldots, m_{10}^{(k)} \sim N(M_k, I_2)$.
- For $i = 1, \ldots, n$, choose $j \in \{1, \ldots, 10\}$ uniformly at random, then draw

$$x_i | y_i \sim N(m_j^{(y_i)}, I_2/5).$$

We take $n = 300$ in this case, with 100 points in each class.