CS578/STAT590: Introduction to Machine Learning **Fall 2014**

Problem Set 3

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1 Questions

1. Fitting an SVM classifier by hand (source: Machine Learning, a probabilistic perspective. K Murphy)

   (a) Write down a vector that is parallel to the optimal vector w.
   The decision boundary is perpendicular to the vector $\phi(x_2) - \phi(x_1)$.

   $$\phi(x_2) - \phi(x_1) = [1, 2, 2]^T - [1, 0, 0]^T = [0, 2, 2]^T$$

   Thus, the vector that is parallel to the optimal vector w is $[0, 1, 1]^T$.

   (b) What is the value of the margin that is achieved by this w?
   The maximum margin is the half of the distance between two points in the 3d feature space. Thus,

   $$\frac{\|\phi(x_2) - \phi(x_1)\|}{2} = \frac{\|[0, 2, 2]^T\|}{2} = \sqrt{2}$$

   (c) Solve for w, using the fact the margin is equal to $1/\|w\|$.
   Let $w = k[0, 1, 1]^T$. Then,

   $$\|w\| = k\|[0, 1, 1]^T\| = \sqrt{2}k$$

   Since the margin is $\sqrt{2}$,

   $$\sqrt{2} = \frac{1}{\|w\|} = \frac{1}{\sqrt{2}k}$$

   By solving this, we obtain $k = 1/2$. Thus, $w = [0, 1/2, 1/2]^T$.

   (d) Solve for w_0 using your value for w and Equations 1 to 3.
   By substituting w of Equations 2 and 3, we get

   $$\begin{cases} y_1(w^T\phi(x_1) + w_0) = -([0, 1/2, 1/2]^T \cdot [1, 0, 0]^T + w_0) = -w_0 \geq 1 \\ y_2(w^T\phi(x_2) + w_0) = ([0, 1/2, 1/2]^T \cdot [1, 2, 2]^T + w_0) = 2 + w_0 \geq 1 \end{cases}$$

   By solving this, we obtain

   $$-1 \leq w_0 \leq -1$$

   Thus, $w_0 = -1$.

(e) Write down the form of the discriminant function $f(x) = w_0 + w^T\phi(x)$ as an explicit function of x.

$$f(x) = w_0 + w^T\phi(x) = -1 + [0, 1/2, 1/2]^T \cdot [1, \sqrt{2}x, x^2]^T = \frac{1}{2}x^2 + \frac{1}{\sqrt{2}}x - 1$$

2. We define a concept space C that consists of the union of k disjoint intervals in a real line. A concept in C is represented therefore using $2k$ parameters: $a_1 \leq b_1 \leq a_2 \leq b_2 \leq \cdots \leq a_k \leq b_k$. An example (a real number) is classified as positive by such concept iff it lies in one of the intervals. Give the VC dimension of H (and prove its correctness).

   The answer is $2k$.

   Proof:

   Let $VC(k)$ be the VC dimension for k disjoint intervals in a real line. I prove by indiction that $VC(k) = 2k$ in the following. When $k = 1$, two examples have four patterns in total, and all the cases can be correctly classified (Figure 1). Thus, $VC(1) = 2$, which satisifies the above hypothesis.

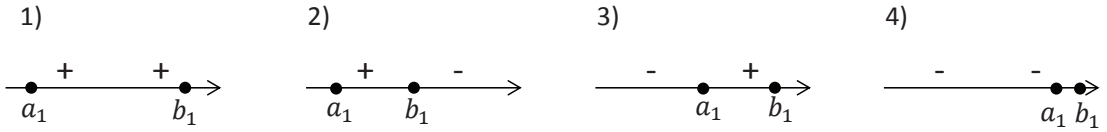

Figure 1: For the case of $k = 1$, two examples are correctly classified in all the four cases. Thus, $VC(1) = 2$.

   Now, given that $VC(k-1) = 2(k-1)$, we want to show that two additional examples can be correctly classified by an additional interval. Assume without loss of generality that two additional numbers are greater than the existing $2(k-1)$ ones that are already classified. Then, there are only four cases in terms of the labels of two additional examples, and they are correctly classified by k-th interval in all cases (Figure 2).

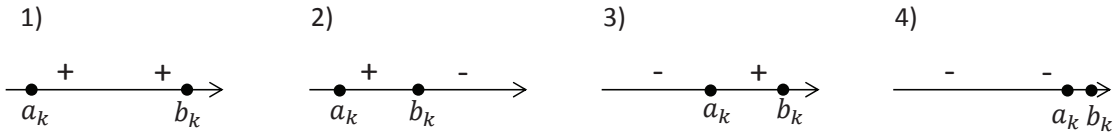

Figure 2: When adding k-th interval, two additional examples are correctly classified in all the four cases.

   Thus,

$$VC(k) \geq VC(k-1) + 2 = 2(k-1) + 2 = 2k$$

   Therefore, $VC(k)$ is at least $2k$ by induction. Also, Figure 3 shows a case in which $k+1$ positive examples and k negative examples cannot be correctly classified. This concludes $VC(k) = 2k$.

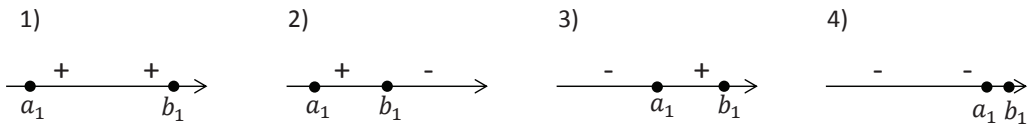

Figure 3: This figure shows a case in which $k+1$ positive examples and k negative examples cannot be correctly classified by k disjoint intervals. The right most positive example (red color) is classified incorrectly. Thus, $VC(k) < 2k + 1$.

3. The Gradient Descent (GD) algorithm

   (a) Write in one sentence: what are the hyper parameters of the GD algorithm.

   The hyper parameters are the initial weight vector which you can randomly initialize if you want, learning rate that is the step size of updating the weight vector, a parameter λ that defines the impact of the regularizer, and the convergence criteria when to stop the iteration such as the maximum number of iterations.

   (b) Write in one sentence: What is the difference between $l1$ and $l2$ regularization.

   $l1$ regularization uses $l1$ norm of w as the regularization term, which encourages the sparsity, while $l2$ regularization uses $l2$ norm of w.

   (c) Write down the gradient descent algorithm applied to hinge loss with $l2$ regularization.

   The objective function is

$$F(w) = \frac{\lambda}{2}\|w\|^2 + \sum_i \max\left(0, 1 - y_i(w^T x_i + b)\right)$$

   Then, its partial derivative with regard to w and b are

$$\frac{\partial F(w)}{w} = \lambda w + \sum_i \begin{cases} -y_i x_i & (\text{if } y_i(w^T x_i + b) \leq 1) \\ 0 & \text{Otherwise} \end{cases}$$

   and

$$\frac{\partial F(w)}{b} = \sum_i \begin{cases} -y_i & (\text{if } y_i(w^T x_i + b) \leq 1) \\ 0 & \text{Otherwise} \end{cases}$$

   The algorithm is shown in Algorithm 1. Note that the bias term is included in the weight vector by extending the feature vector as $[x, 1]^T$ and the weight vector as $[w, b]^T$.

2 Programming Assignment

For the programming assignment, I used SVM with the hinge loss function and $l1$ or $l2$ regularization as required. The pseudo code of gradient descent algorithm to solve this is shown in Algorithm 2, which is basically similar to Algorithm 1 except that both $l1$ and $l2$ are supported.

Algorithm 1 Gradient descent algorithm applied to hige loss with l2 regularization

procedure HINGEREGULARIZEDGD()
  $w = (0, \cdots, 0)$
  $b = 0$
  for $i = 0$ to $maxIterations$ **do**
    $\Delta w = (0, \cdots, 0)$
    $\Delta b = 0$
    for all training data (x_d, y_d) for $d = 1, \cdots, D$ **do**
      if $y_d(w \cdot x_d + b) \leq 1$ **then**
        $\Delta w = \Delta w + y_d x_d$
        $\Delta b = \Delta b + y_d$
    $\Delta w = \Delta w - \lambda w$
    $w = w + \eta \Delta w$
    $b = b + \eta \Delta b$
  return w and b

Algorithm 2 Gradient descent algorithm applied to hige loss with l1 and l2 regularization

procedure GD(MAXITERATIONS, REGULARIZATION, η, λ)
  $w = (0, \cdots, 0)$
  $b = 0$
  for $iter = 0$ to $maxIterations$ **do**
    $\Delta w = (0, \cdots, 0)$
    $\Delta b = 0$
    for all training data (x_d, y_d) for $d = 1, \cdots, D$ **do**
      if $y_d(w \cdot x_d + b) \leq 1$ **then**
        $\Delta w = \Delta w + y_d x_d$
        $\Delta b = \Delta b + y_d$
    if regularization == $l1$ **then**
      for $i = 0$ to N **do**
        if $w_i \geq 0$ **then**
          $\Delta w_i = \Delta w_i - \lambda$
        else
          $\Delta w_i = \Delta w_i + \lambda$
    else if regularization == $l2$ **then**
      $\Delta w = \Delta w - \lambda w$
    $w = w + \eta \Delta w$
    $b = b + \eta \Delta b$
  return w and b

Feature Set

For the continuous values, I used all the intervals between two consequtive thresholds as attributes. For instance, if an original attribute a has three thresholds $1, 2, 3$, then the corresponding attributes will be $\{(a < 1), (a \geq 1; a < 2), (a \geq 2; a < 3), (a \geq 3)\}$. Also, I ignored the examples that contain missing values.

Hyper Parameters

There are five hyper parameters, *maxIterations*, $l1$ or $l2$, *stepSize*, *lambda*, and feature set. Unlike Perceptron algorithm, we want to minimize the objective function without worrying about overfitting because the regularization term somewhat avoids it. Thus, I used a very large number for maxIterations, say 20000, to get the gradient descent converged. For instance, Figure 4 shows the decrease of the objective function over the steps when $stepSize = 0.0001$ and $labmda = 0.01$. This shows that $maxIterations = 20000$ is enough to converge even for a very small *stepSize*.

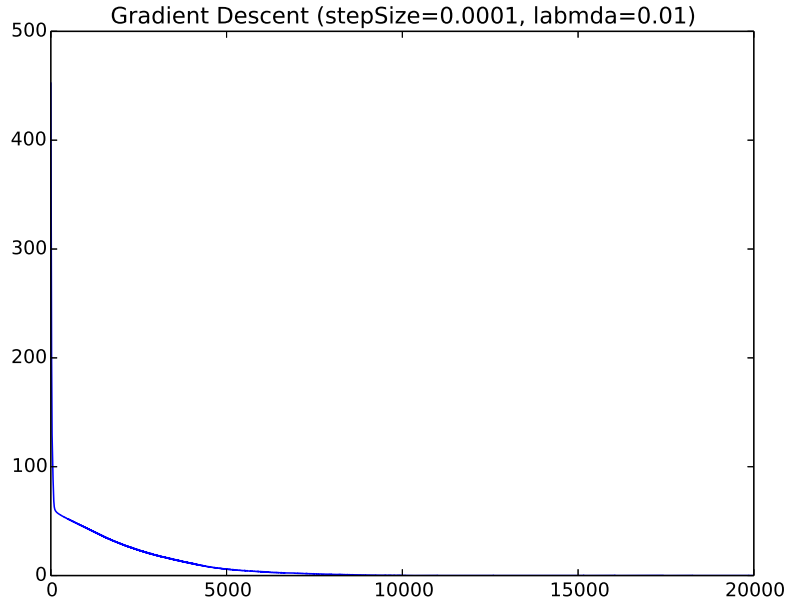

Figure 4: This figure shows the descrese of the objective over the steps when $stepSize = 0.0001$ and $labmda = 0.01$.

For other hyperparameters, I employed a kind of brute-force approach to find the best ones. For each combination of *regularization* and $featureSet$, I tried all the combination of $stepSize \in \{0.0001, 0.001, 0.01, 0.1\}$ and $labmda \in \{0.001, 0.001, 0.01, 0.1, 1\}$ in order to find the best ones. The results are shown in Table 1.

featureSet	regularization	best stepSize	best lambda
1	11	0.1	0.001
1	12	0.1	0.01
2	11	1	0.0001
2	12	1	0.0001
3	11	1	0.0001
3	12	1	0.0001

Table 1: The best combination of *stepSize* and *lambda*

Results

Using the best combination of hyperparameters, the classifier was learned and the performance was evaluated against the test data. The results are shown in Figures ?-?.

dataset	accuracy	precision	recall	F1
training data	?	?	?	?
validation data	?	?	?	?
test data	?	?	?	?

Table 2: The results of featurSet=1 with $l1$ regularization

dataset	accuracy	precision	recall	F1
training data	0.967	0.966	0.961	0.963
validation data	0.967	0.931	1.0	0.964
test data	0.598	0.568	0.819	0.671

Table 3: The results of featurSet=1 with $l1$ regularization

Notice that the accuracy on the training data is not 1.0. This is mainly because of the regularization term that avoids overfitting.

*** The regularizers $l1$ and $l2$ have different impact on the results. .... In general, $l1$ has weigh more on the significant attributes. In our dataset, this works better than $l2$.....

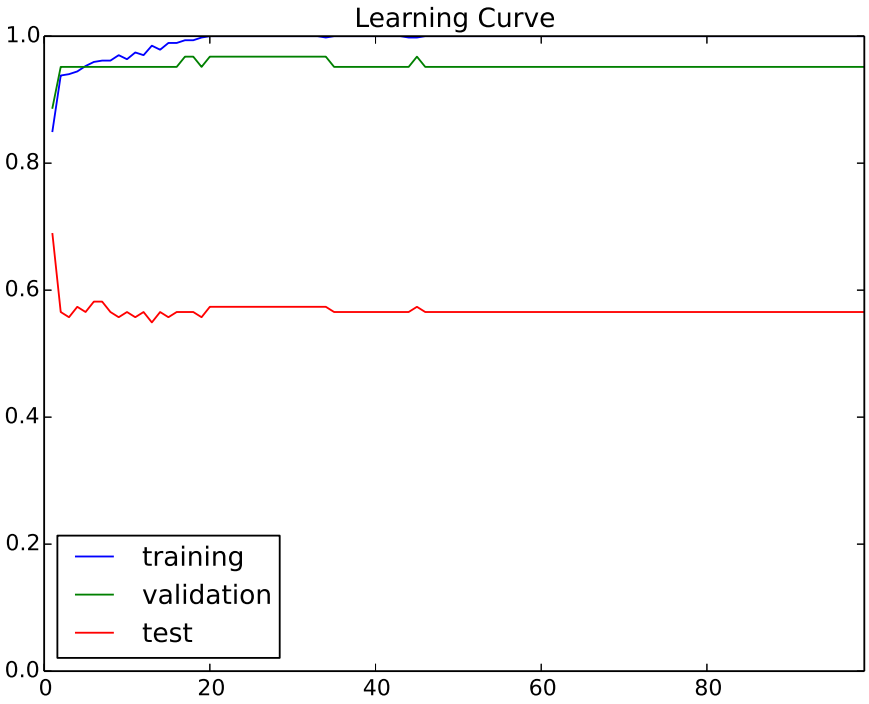

Figure 5: This figure shows the learning curve with $l2$ regularization and $featureSet = 1$.