### 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

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

By solving this, we obtain

$$-1 \le w_0 \le -1$$

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:  $a_1 \le b_1 \le a_2 \le b_2 \le \cdots \le a_k \le b_k$ . 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 satisfies the above hypothesis.

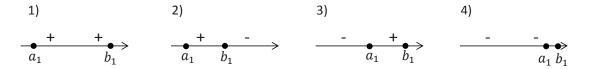


Figure 1: For the case of k = 1, two examples are correctly classified in all the four cases. Thus, VC(1) = 2.

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).

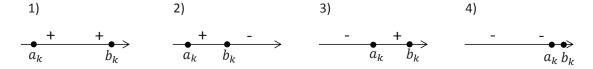


Figure 2: When adding k-th interval, two additional examples are correctly classified in all the four cases.

Thus,

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

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. Thus, VC(k) < 2k+1. This concludes VC(k) = 2k.

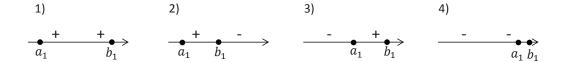


Figure 3: This figure shows a case in which k+1 positive examples and k negative examples cannot be correctly classified by k disjoint intervals. The right most positive example (red color) is classified incorrectly. Thus, VC(k) < 2k + 1.

#### 3. The Gradient Descent (GD) algorithm

- (a) Write in one sentence: what are the hyper parameters of the GD algorithm. The hyper parameters are 1) how to define the initial parameters: initializing 0 or randomly, 2) the learning rate that is the step size of updating the parameters, and 3) the convergence criteria when to stop the iteration such as the maximum number of iterations and a threshold to judge whether it is coverged.
- (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 and leads to a simpler model, while l2 regularization uses l2 norm of w.
- (c) Write down the gradient descent algorithm applied to hinge loss with l2 regularization.

#### Algorithm 1 Gradient descent algorithm applied to hige loss with 12 regularization

```
1: procedure HingeRegularizedGD()
 2:
         w = (0, \cdots, 0)
 3:
         b = 0
 4:
         for i = 0 to maxIterations do
             \Delta w = (0, \cdots, 0)
 5:
             \Delta b = 0
 6:
             for all training data (x_d, y_d) for d = 1, \dots, D do
 7:
                 if y_d(w \cdot x_d + b) \leq 1 then
 8:
                      \Delta w = \Delta w + y_d x_d
 9:
                      \Delta b = \Delta b + y_d
10:
             \Delta w = \Delta w - \lambda w
11:
             w = w + \eta \Delta w
12:
             b = b + \eta \Delta b
13:
         return w and b
14:
```

The objective function is

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

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

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

and

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

The algorithm is shown in Algorithm 1.

## 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 2 Gradient descent algorithm applied to hige loss with 11 and 12 regularization
```

```
1: procedure GD(MAXITERATIONS, REGULARIZATION, \eta, \lambda)
         w = (0, \cdots, 0)
 2:
 3:
         b = 0
 4:
         for iter = 0 to maxIterations do
             \Delta w = (0, \cdots, 0)
 5:
             \Delta b = 0
 6:
 7:
             for all training data (x_d, y_d) for d = 1, \dots, D do
                 if y_d(w \cdot x_d + b) \leq 1 then
 8:
                      \Delta w = \Delta w + y_d x_d
 9:
                      \Delta b = \Delta b + y_d
10:
             if regularization == l1 then
11:
                 for i = 0 to N do
12:
                      if w_i \geq 0 then
13:
                          \Delta w_i = \Delta w_i - \lambda
14:
                      else
15:
                          \Delta w_i = \Delta w_i + \lambda
16:
             else if regularization == l2 then
17:
                  \Delta w = \Delta w - \lambda w
18:
             w = w + \eta \Delta w
19:
20:
             b = b + \eta \Delta b
21:
             return w and b if they are converged
        return w and b
22:
```

#### 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  $\{(a < 1), (a \ge 1; a < 2), (a \ge 2; a < 3), (a \ge 3)\}$ . 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 takes care of it. Thus, I used a very large number for maxIterations, say 20000, to get the gradient descent converged. Also, as it is shown in Algorithm 2, I checked the decrease in the objective function during the gradient descent and if it is within the threshold, the gradient descent stops. I used 0.0001 as threshold. Figure 4 (featureSet = 1, stepSize = 0.001, and labmda = 0.4) and 5 (featureSet = 2, stepSize = 0.001, and labmda = 1.0) show the decrease of the objective function over the iterations. A large stepSize leads to more oscillation while a small stepSize requires a large number of iterations to converge. The result of Figure 4 indicates that maxIterations = 20000 is enough to converge even for a very small stepSize for this problem.

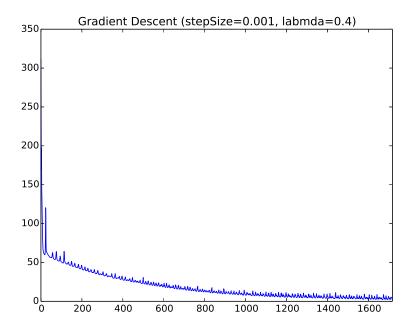


Figure 4: This figure shows the descrese of the objective over the iterations when featureSet = 1, stepSize = 0.001, and labmda = 0.4.

For stepSize and lambda, I employed a brute-force approach to find the best values. For each combination of regularization and featureSet, I tried all the combination of  $stepSize \in \{0.001, 0.01, 0.1\}$  and  $labmda \in \{0.05, 0.1, 0.2, 0.4, 1.0, 2.0\}$  in order to find the optimal values

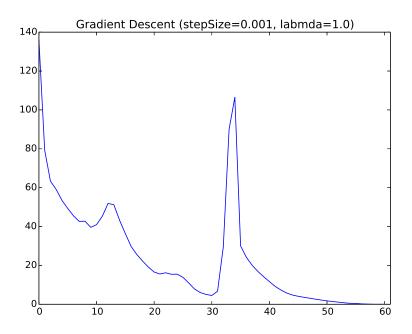


Figure 5: This figure shows the decrese in the objective over the iterations when featureSet = 2, stepSize = 0.001, and lambda = 1.0.

that achieve the best accuracy on the validation data. One of the results are shown in Figure 6. Notice that the performance significantly decreases when  $lambda \geq 1$ . This is resonable because the loss function becomes less important in the objective function. A large lambda avoids overfitting but may deteriorate the performance, while a small lambda can achieve better performance but may results in overfitting. Since we do not know the distribution of the test dataset beforehand, it is reasonable to use the performance on the validation data to choose values of labmda as well as other hyperparameters. Note that if the distribution of the test dataset is significantly different from the validation dataset, then the selected values of hyperparameters cannot necessarily yield a good performance on the test dataset.

The optimal values of stepSize and labmda that achieved the best performance on the validation data are listed in Table 1. For the following performance test, I used those values for hyperparameters.

featureSet	regularization	best stepSize	best lambda
1	11	0.001	0.4
1	12	0.001	0.4
2	11	0.001	0.1
2	12	0.001	0.2
3	11	0.001	0.05
3	12	0.001	0.1

Table 1: The best combination of stepSize and lambda

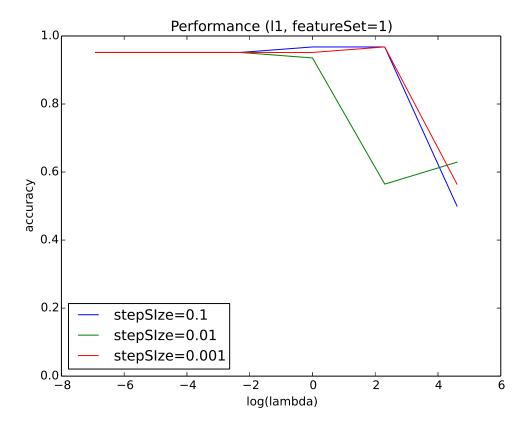


Figure 6: This figure shows the accuracy over the validation data using different pairs of stepSize and lambda when regularization = l2 and featureSet = 1. The performance drastically decreases when lambda > 1.

#### Results

Using the selected values of stepSize and lambda for each featureSet and regularization, the classifier was learned and the performance was evaluated on the training, validation, and test dataset. The results are shown in Tables 2-7. Note that the performance of featureSet = 2 is very close to the one of featureSet = 3. This implies that the feature pairs have much larger weighs than the original attributes when featureSet = 3 is used. Also, it is surprising that featureSet = 1 yields the best performance. The possible reason is that the feature pairs cause the overfitting even though the regularizer is included in the objective.

dataset	accuracy	precision	recall	F1
training data	1.0	1.0	1.0	1.0
validation data	0.967	0.931	1.0	0.964
test data	0.614	0.583	0.803	0.675

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

dataset	accuracy	precision	recall	F1
training data	0.989	0.990	0.985	0.987
validation data	0.967	0.931	1.0	0.964
test data	0.598	0.571	0.786	0.662

Table 3: The results of featurSet=1 with l2 regularization

dataset	accuracy	precision	recall	F1
training data	1.0	1.0	1.0	1.0
validation data	0.967	0.931	1.0	0.964
test data	0.590	0.560	0.836	0.671

Table 4: The results of featurSet=2 with l1 regularization

dataset	accuracy	precision	recall	F1
training data	1.0	1.0	1.0	1.0
validation data	0.967	0.931	0.1.0	0.964
test data	0.606	0.573	0.836	0.680

Table 5: The results of featurSet=2 with l2 regularization

## Impact by the regularizer l1 and l2

In general, l1 regularizer results in a sparse weight vector compared to l2 regularizer. To confirm this, for featureSet = 1 I normalized the resulting weight vectors and compare

dataset	accuracy	precision	recall	F1
training data	1.0	1.0	1.0	1.0
validation data	0.967	0.931	1.0	0.964
test data	0.606	0.573	0.836	0.680

Table 6: The results of featurSet=3 with l1 regularization

dataset	accuracy	precision	recall	F1
training data	1.0	1.0	1.0	1.0
validation data	0.967	0.931	1.0	0.964
test data	0.606	0.573	0.836	0.680

Table 7: The results of featurSet=3 with l2 regularization

them between l1 and l2. Out of 586 components of the weight vector, 313 components are zero when l1 regularizer is used, while only 287 componets are zero when l2 regularizer is used. This result confirms that l1 regularizer leads to a sparse weight vector. The sparsity is usually favorable because it leads to a simpler model, which indicates a more generalized model and requries less storage. Although it is known that l1 regularizer often leads to better performance in practice, there is usually not a considerable difference between the two methods in terms of the accuracy of the resulting model [1, 2]. In fact, there is no significant difference in performace between l1 and l2 in the results.

## References

- [1] Gao, J., Andrew, G., Johnson, M., Toutanova, K. 2007. A comparative study of parameter estimation methods for statistical natural language processing. In *Proceedings of ACL*, pp. 824 831.
- [2] Tsuruoka, Y., Tsujii, J., Ananiadou, S. 2009. Stochastic gradient descent training for l1-regularized log-linear models with cumulative penality. In *Proceedings of ACL*, pp. 477 485.