# Machine Learning 6.867 - Pset 2

October 23, 2015

## 1 Logistic Regression

### 1.1 Implementation

We implemented $L_2$-regularized logistic regression using gradient descent. The objective function to be minimized over is:

$$\sum_{i=1}^{n} \log(1 + e^{-y^{(i)}(\mathbf{w}^T\mathbf{x}^{(i)}+w_0)}) + \lambda \mathbf{w}^T\mathbf{w} \tag{1}$$

We used both our implementation of gradient descend and the `Matlab` function `fminunc`. Convergence criterion is reached within reasonable iterations in both implementations.

### 1.2 Testing in data with $\lambda = 0$

We run the logistic regression on the four data sets, setting the regularization parameter $\lambda = 0$. The estimated coefficients are listed in Table 1.

Table 1: Estimated logistic regression coefficients and accuracy, $\lambda = 0$

| Data | $w_0$ | $w_1$ | $w_2$ | Training accuracy | Validation accuracy |
|---|---|---|---|---|---|
| stdev1 | -66.3378 | 95.2461 | 101.1527 | 1.0000 | 1.0000 |
| stdev2 | -0.0466 | 0.7636 | 1.1148 | 0.9075 | 0.9200 |
| stdev4 | -0.0093 | 0.2363 | 0.2034 | 0.7400 | 0.7525 |
| nonsep | 0.0006 | -0.0247 | -0.0237 | 0.5150 | 0.4925 |

The decision boundaries at various thresholds are plotted in Figure 1. We observe the following phenomenon:

1. As data become more linearly non-separable, the accuracy is lower, and the decision boundary has higher variance with respect to data (for example, as $\sigma$ increases, the decision boundary and accuracy are more different between training and validation.)

2. As data become more linearly non-separable, the estimated logistic function is also less steep, reflected in the wider bands in the plots and lower norm of $\mathbf{w}$. This is reasonable because the classifier is not as certain about how to classify the data points in the mix zone.

3. In the totally non-separable case, logistic regression fails to classify, barely reaching the 50% baseline.

### 1.3 Testing in data with positive $\lambda$

Similarly, we run logistic regression with other values of $\lambda$. In particular, we use the cross-validation technique to select best value of $\lambda$ using the validation set accuracy. In particular, for the four datasets, we choose $\lambda = 0$, $\lambda = 0$, $\lambda = 10$, and $\lambda = 10$ respectively.

## 2 Support Vector Machine

Support Vector Machines are a popular classification method to construct linear or nonlinear decision boundaries by solving a convex optimization problem. There are two common forms of the optimization problem considered for SVM, which we refer to as the primal and dual. In this paper, we only consider the dual form, because it is computationally more tractable for many problems, and this method has the ability to generalize to different choices of kernel. The dual form of SVM for a general kernel function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is as follows:

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^n} \quad & \sum_{i=1}^{n} \alpha_i - \tfrac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} k(x^{(i)}, x^{(j)}) \\ \text{s.t.} \quad & 0 \le \alpha_i \le C, \qquad\qquad i = 1, \dots, n, \\ & \sum_{i=1}^{n} \alpha_i y^{(i)} = 0. \end{aligned} \tag{2}$$

### 2.1 Implementation

First, we implemented the dual form of the SVM with a linear kernel, where $k$ is the usual dot product $k(x, z) = \langle x, z \rangle$ for all $x, z \in \mathcal{X}$. In MATLAB, we created a function with inputs: data $X \in \mathbb{R}^{n \times p}$, labels $Y \in \{-1, 1\}$, and cost parameter $C \in \mathbb{R}^+$. Within the function, we use the quadratic solver `quadprog` to solve the SVM dual problem (2) with these parameters to find the optimal $\alpha$'s. Since `quadprog` requires that the problem fit into a certain functional form, we reformulate the problem (2) as follows:

$$\begin{aligned} -\min_{\alpha \in \mathbb{R}^n} \quad & \tfrac{1}{2} \alpha^T H \alpha - \sum_{i=1}^{n} \alpha_i \\ \text{s.t.} \quad & 0 \le \alpha_i \le C, \qquad i = 1, \dots, n, \\ & \sum_{i=1}^{n} \alpha_i y^{(i)} = 0, \end{aligned} \tag{3}$$

where: $H \in \mathbb{R}^{n \times n}$ is a matrix with $(i, j)^{th}$ entry $H_{ij} = y^{(i)} y^{(j)} k(x^{(i)}, x^{(j)})$. Given the optimal solution $\alpha \in \mathbb{R}^n$ for the SVM problem with a linear kernel, the chosen linear decision boundary $\theta^T x + \theta_0 = 0$ is given by:

$$\theta = \sum_{i=1}^{n} \alpha_i y^{(i)} x^{(i)} \tag{4}$$

$$\theta_0 = \frac{1}{\mathcal{M}} \Big( \sum_{j \in \mathcal{M}} \Big( y^{(j)} - \sum_{i \in \mathcal{S}} \alpha_i y^{(i)} (x^{(j)})^T x^{(i)} \Big) \Big) \tag{5}$$

The output of our linear SVM function is $[\theta, \theta_0]$. We tested our function on the 2D example $X = \{(1, 2), (2, 2), (0, 0), (-2, 3)\}$, $Y = \{1, 1, -1, -1\}$. For this problem, the objective function generated for problem (3) is:

$$\frac{1}{2} \alpha^T H \alpha - \sum_{i=1}^{4} \alpha_i, \tag{6}$$

where:

$$H = \begin{bmatrix} 5 & 6 & 0 & -4 \\ 6 & 8 & 0 & -2 \\ 0 & 0 & 0 & 0 \\ -4 & -2 & 0 & 13 \end{bmatrix}$$

The constraints are:

$$0 \le \alpha_i \le C, \quad i = 1, \dots, 4, \tag{7}$$

$$\alpha_1 + \alpha_2 - \alpha_3 - \alpha_4 = 0. \tag{8}$$

### 2.2 Performance on datasets

We tested our linear SVM function on the same 2D datasets from the previous section, with parameter $C = 1$.

### 2.3 Kernel SVM

We extended our SVM implementation in MATLAB to operate with more general kernels, taking the kernel function or kernel matrix as input.

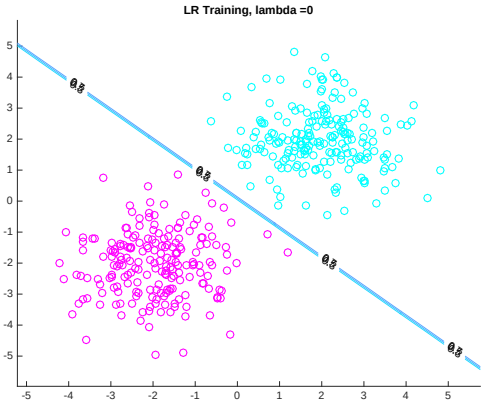
**Questions:**

(a) As $C$ increases, the geometric margin $1/\|\mathbf{w}\|$ decreases. If the data is not linearly separable, then the geometric margin $1/\|\mathbf{w}\|$ decreases strictly monotonically as $C$ increases. However, if the data is linearly separable, then this does not always happen as we increase $C$. In this case, once the margin is sufficiently small such that all points are correctly classified, then it will not decrease further even as $C$ approaches infinity.

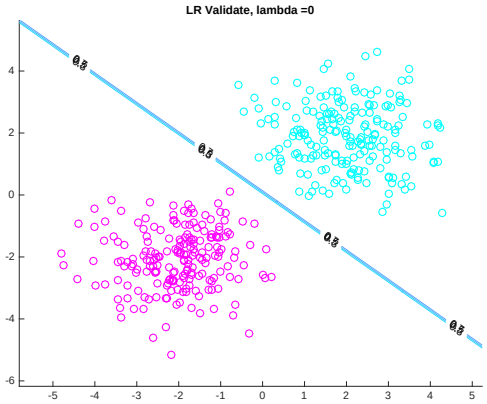
(b) As $C$ decreases, the number of support vectors decreases. This is because the larger penalty on misclassified points leads to a decision boundary with fewer misclassifications on the training data. However, the number of the support vectors is bounded below by two as $C$ approaches infinity, because there will always be at least one support vector on each side of the decision boundary.

(c) Maximizing the geometric margin $1/\|\mathbf{w}\|$ on the training data is not an appropriate criterion for selecting $C$ because this leads to a classifier which is overfit to the training set. To obtain a classifier which generalizes well on test data, we should use out-of-sample data to select an appropriate value for $C$. To do this, we can train the SVM model with $C = \{0.01, 0.1, 1, 10, 100\}$, and then select the value for $C$ which yields the classifier with the highest accuracy on the validation set.

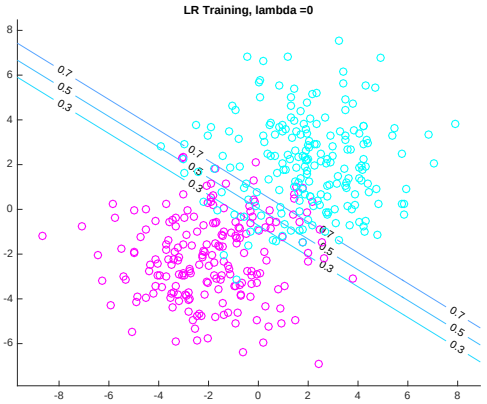
## 3 Titanic Data



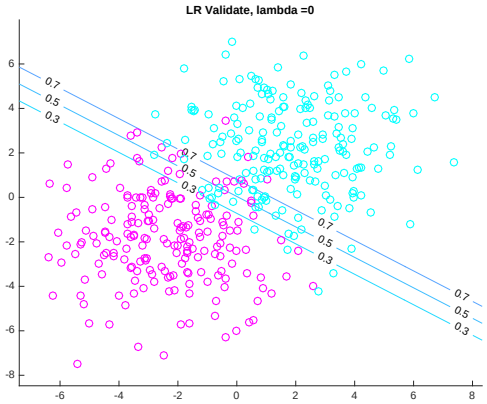

(a) Data with $\sigma = 1$, training



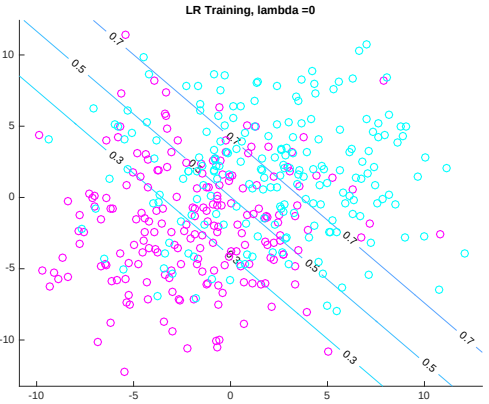

(b) Data with $\sigma = 1$, validation



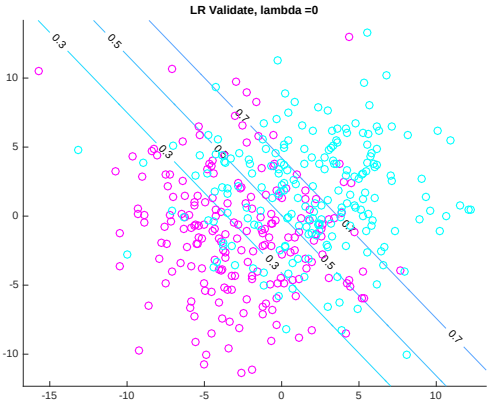

(c) Data with $\sigma = 2$, training



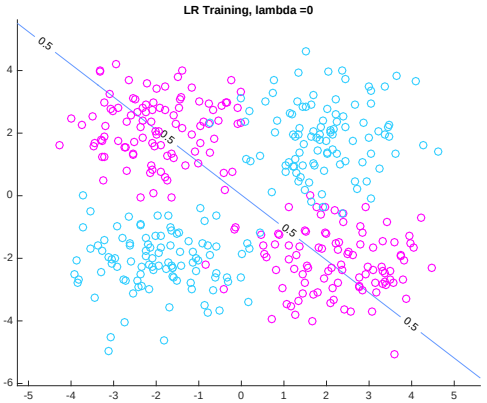

(d) Data with $\sigma = 2$, validation



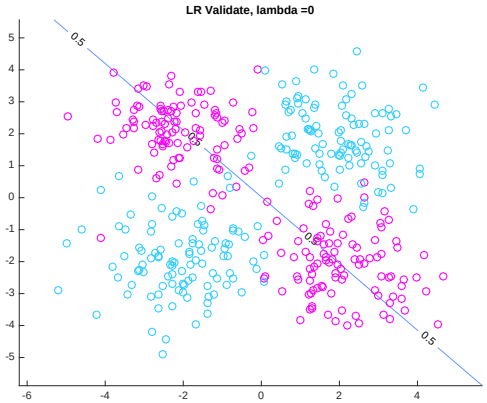

(e) Data with $\sigma = 4$, training




(f) Data with $\sigma = 4$, validation




(g) Non-seperable data, training




(h) Non-seperable data, validation