Machine Learning 6.867 - Pset 1

October 1, 2015

1 Implement Gradient Descent

1.1 Implementation

We implemented a basic gradient descent function in MATLAB. In this function, the user can specify the objective function and the corresponding gradient function. User also specify initial guess, the constant step size, and the convergence threshold.
The procedure works as the following: starting at the initial guess, we move to a new point by taking a step (of the specified step size) in the direction of the gradient. We repeat the process until the objective values between two iterations are less than the specified threshold.

1.2 Testing Gradient Descent

We test the gradient descent procedure in the following functions:

1. $f(x_1, x_2) = 3x_1^2 + 2x_1x_2 + x_2^2 - 4x_1 + 5x_2$ (By completing the square we get the optimal value is at $x_1 = 2.25, x_2 = -4.75$.)
2. $f(x) = -\frac{1}{\sqrt{2\pi}\sigma}e^{-(x-\mu)^2/2\sigma^2}$ (negative of a Gaussian pdf, with $\mu = 0$ and $\sigma = 1$.)
3. $f(x) = x^3 - 10x$. (This is not a convex function; local minimum is at 1.8257 and global minimum is negative infinity).

The basic gradient descent method works decently well in the first two functions. In most specifications of the initial guess and step size the procedure converges to the right answer. Changing the convergence threshold to very large gives imprecise results, and changing it to very small results in more iterations until convergence. In some cases, very large or very small step sizes may result in non-convergence. In the third function which is non-convex, the initial guess can lead us to the incorrect, local minimum.

1.3 Numerical Gradient

We can also numerically evaluate the gradient at a given point. The partial derivative at x_i is evaluated by taking the difference between $f(\mathbf{x} + \mathbf{h})$ and $f(\mathbf{x} - \mathbf{h})$, where $\mathbf{h}$ is the vector of all zeros except for the ith component being ϵ, and divide the difference by 2ϵ. We apply this numerical gradient in place of the analytic one in the original three functions, and found that for sufficiently small ϵ, the results are almost identical!

1.4 Comparing with Sophisticated Methods

As the final step to evaluate our implementation of gradient descent, we would like to compare ours with the more developed methods. Comparing with `fminunc`, our implementation is dramatically slower, unfortunately. For example, for the same convergence criterion, it takes 8 iterations for `fminunc` to converge, whereas it takes

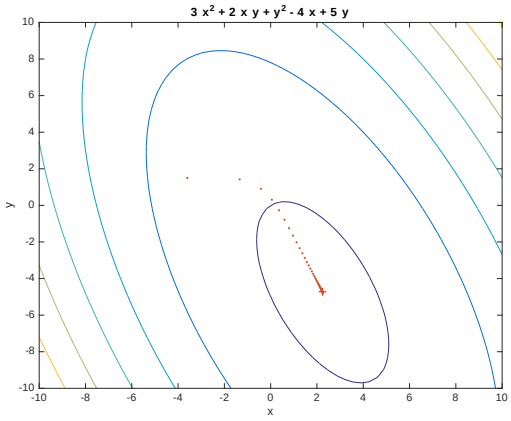


Figure 1: Contour plot of the first function. The gradient descent method moves along the red dots in the steps toward the red cross where the local/global optimal is.

35 iterations for our method. We think the disadvantage is from our constant step size. Since this size does not adapt to where we are, our method is likely to undershoot or overshoot. An improvement could be using backtracking, exact line-search, etc. methods to adaptively update the step size.

2 Linear Basis Function Regression

2.1 MLE for Polynomial Basis Function Regression

We implemented a maximum likelihood estimator for a linear regression with polynomial basis functions, using the formula $\mathbf{w} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$. The replicated weight vectors are close to what is reported in Table 1.1, and the plots we generated in Figure 2a match the ones in Bishop well:

2.2 Using SSE

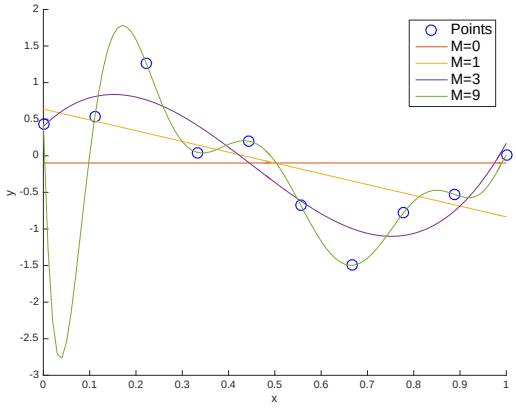
Alternatively, the maximum likelihood weight vector can be found using numerical gradient descent on the SSE. We first implement code to calculate the SSE: $(\mathbf{Y} - \mathbf{\Phi w})'(\mathbf{Y} - \mathbf{\Phi w})$. The derivative is $-2\mathbf{\Phi}(\mathbf{Y} - \mathbf{\Phi w})$, or can be computed numerically using the finite differencing method we implemented in Problem 1. We found that the two match.

2.3 Use Gradient Descent on SSE to find MLE

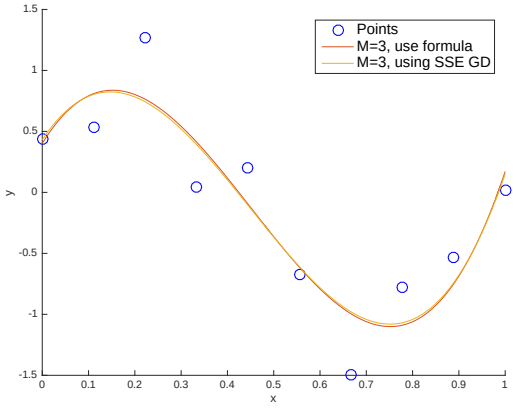
To get MLE for $\mathbf{w}$, we feed the SSE as the objective function in the gradient descend, $\mathbf{w}$ as the variable to be optimized over. With some smart initial guess, step size, and reasonably small convergence threshold, our $\mathbf{w}$ from gradient descent match the analytic solution using the formula largely (but not exactly). The comparison can be found in Figure 2b. Some bad choice of step size results in non-convergence or extremely large estimates.

2.4 Sine Basis Function

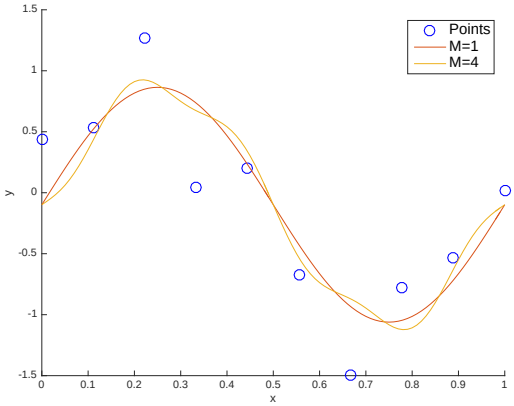
We can also use sine basis functions, with $\phi_1(x) = \sin(2\pi x), \ldots, \phi_M(x) = \sin(2\pi M x)$. The estimated plots are in Figure 2c. We observe that the estimated function is not only periodic at period equal to one, for larger values of M it is even periodic within a period! Potential disadvantage is that the data is assumed to be periodic.



(a) Replication of Bishop 1.4, using polynomial basis function up to degree M.



(b) Comparing the estimates using MLE equation or numeric gradient descent on SSE.



(c) Using sine basis function.

Figure 2

3 Ridge Regression

3.1 Implementation

Ridge regression is the particular case of regularized least squares with a quadratic regularizer term. The error function that we aim to minimize over is given by:

$$\frac{1}{2}\sum_{n=1}^{N}(t_n - \mathbf{w}^T\phi(\mathbf{x}_n))^2 + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w} \tag{1}$$

The closed-form solution of this problem is well-known, and can be derived by setting the gradient of (3) equal to zero. The optimal solution for $\mathbf{w}$ is provided by Bishop (2006), page 145:

$$\mathbf{w}_{ridge} = (\lambda\mathbf{I} + \Phi^T\Phi)^{-1}\Phi^T\mathbf{t} \tag{2}$$

We coded this method in MATLAB and tested our program using data from Bishop Figure 1.4, varying the parameters of λ and M. For the extreme cases, we observed that if $\lambda \leq 0.0001$, then $\mathbf{w}_{ridge} \approx \mathbf{w}_{OLS}$, and if $\lambda \geq 100$, then $\mathbf{w}_{ridge} \approx \mathbf{0}$.

3.2 Model Selection

To optimize parameter values for λ and M, we build our models using training data and then compare out-of-sample performance on validation data. For this example, we performed a grid search over the ranges: $\lambda = \{0.0001, 0.001, 0.01, 0.1, 1, 10, 100\}$, $M = \{0, 1, 2, 3, 4, 5\}$. We found that the model with $\lambda =$ TODO and $M =$ TODO yields the lowest MSE on validation data, so we select these to be the final parameter values. This model leads to MSE = TODO for the test data, which is the TODO lowest overall. In general, we observe that models with MSE for the validation set tend to yield low MSE on the test set.

4 Sparsity and LASSO

An alternative approach is to use the L_1 norm regularizer in the objective for regularized least squares. The error function that we aim to minimize over is given by:

$$\frac{1}{N}\sum_{n=1}^{N}(t_n - \mathbf{w}^T\phi(\mathbf{x}_n))^2 + \frac{\lambda}{2}\sum_{j=1}^{M}|w_j| \tag{3}$$

The LASSO is widely used in practice because it leads to solutions which are relatively sparse, i.e. the resulting prediction vector $\mathbf{w}$ tends to have few non-zero components.

To test this method and its sparsity properties, we consider a regression problem with 5 training points and 500 testing points in $\mathbb{R}^{12}$. The data is generated according to $f(x) = \mathbf{w}^T\phi(\mathbf{x}) + \epsilon$, where $\epsilon \sim N(0, \sigma^2)$ and $\mathbf{w} \in \mathbb{R}^{12}$ is a sparse vector with only two non-zero components. For this problem, we assume that $\mathbf{w}$ is unknown, and we estimate this vector with ridge regression in Section 4.1 and with LASSO in Section 4.2. Let λ_2 denote the regularizer term for the L_2 norm and let λ_1 denote the regularizer term for the L_1 norm. Figure **??** shows plots of the estimated function with different regularizers.

4.1 Ridge Regression Gradient Descent

Applying our method for gradient descent to the ridge regression problem on the training dataset of 12 points, we compute the vector of weights $\mathbf{w}$ and MSE on the testing dataset for $\lambda_2 = 0.1$. We obtain:

$$\mathbf{w} = (w_1, w_2, w_3, w_4, w_5, w_6, w_7, w_8, w_9, w_{10}, w_{11}, w_{12}),$$
$$\text{MSE} = TODO.$$

If we disable the L_2 regularizer (set $\lambda_2 = 0$), we obtain:

$$\mathbf{w} = (w_1, w_2, w_3, w_4, w_5, w_6, w_7, w_8, w_9, w_{10}, w_{11}, w_{12}),$$
$$\text{MSE} = TODO.$$

4.2 LASSO Gradient Descent

Similarly, we apply our method for gradient descent to the LASSO problem on the on the training dataset of 12 points. For $\lambda_1 = 0.1$, we find:

$$\mathbf{w} = (w_1, w_2, w_3, w_4, w_5, w_6, w_7, w_8, w_9, w_{10}, w_{11}, w_{12}),$$
$$\text{MSE} = TODO.$$

If we disable the L_1 regularizer (set $\lambda_1 = 0$), we find:

$$\mathbf{w} = (w_1, w_2, w_3, w_4, w_5, w_6, w_7, w_8, w_9, w_{10}, w_{11}, w_{12}),$$
$$\text{MSE} = TODO.$$

4.3 Sparsity Properties of LASSO