6.867 Problem Set 1

October 1, 2015

Problem 1

We implemented a rather naive gradient descent in Python using an algorithm similar to the pseudocode below. The function is written in such a way that it can accept arbitrary scalar functions f and their gradients, $\nabla f(x)$, where x can be a vector of arbitrary length, n. The goal of this function is to try and return $\arg\min_x f(x)$.

Algorithm 1 Gradient Descent

```
procedure GRADIENT DESCENT
    Specify initial guess, step size, and convergence criteria
    Set current guess equal to initial guess
    while Distance between last guess and current guess location is greater than convergence criteria do
        Calculate function at current location
        Calculate the gradient of function at current location
        Updated guess = take a step from current guess in direction of gradient proportional to step size
        Calculate distance between updated guess and current guess
        Set current guess equal to updated guess
    end while
end procedure
```

In order to understand the effect of various hyperparameters (our initial guess, the step size, and the convergence criteria) of the algorithm, we compared the results of our gradient descent routine given a number of different parameter combinations for two different functions: $f(x) = \sum_i^n x_i^2$ and $f(x) = \sum_i^n \frac{1}{100} x_i^2 - \cos(x)$. The first of these is a convex function, whereas the second is quite non-convex, with many local minima. The results of our gradient descent algorithm for numerous values are found below in Table 1.

We find that, in general, the convex function behaves considerably better. Regardless of our initial guess or our learning rate, the algorithm returns a guess in fewer than 1,000 steps, and these guesses are consistently close to $x = (0, 0, 0, 0)$, the "true" value. The final guess' distance from the true value of x is primarily a function of the convergence criteria, which makes sense - the less picky we are with our convergence criteria, the further from the true value of x our final guess will be.

The non-convex function, on the other hand, is much more sensitive to the hyperparameters we specify. The most notable departure from the convex function is the influence of our initial guess. It is much easier for our gradient descent algorithm to get trapped in local minima, and this is clearly illustrated in our results. While this is the most obvious difference, note that changes in both the learning rate and the convergence criteria also lead to non-trivially different guesses for $\arg\min_x f(x)$.

Generally speaking, choice of starting value is only in when were are dealing with non-convex functions as different starting values may lead to different local extremums. Though if we randomly initialized good starting values, it decreases the number of iterations necessary for convergence. Tuning the step size alters the performance of the algorithm, while tuning the convergence threshold alters the accuracy of the algorithm.

To elaborate on this a little, for any given convergence threshold, increasing step size will decrease the number of iterations required for convergence. However, we need make sure that the step isn't so large that the algorithm gets caught in a loop where its constantly overshooting the minimum. On the other hand, for a given step size, decreasing the convergence threshold increases accuracy of the algorithm, but at the

Table 1: Performance of gradient descent given various algorithm hyperparameters

$Guess_i$	step	Thresh.	$Guess_f$ ($f(x) = \sum_i^n x_i^2$)	$Guess_f$ ($f(x) = \sum_i^n \frac{1}{100} x_i^2 - \cos(x)$)
[5.0, -3.0, 7.0, 8.0]	0.3	0.1	[0.020, -0.012, 0.029, 0.033]	[6.150, -0.314, 6.165, 6.176]
[5.0, -3.0, 7.0, 8.0]	0.3	0.001	[0.001, -0.001, 0.002, 0.002]	[6.159, -0.025, 6.160, 6.161]
[5.0, -3.0, 7.0, 8.0]	0.3	1e-05	[0.000, -0.000, 0.000, 0.000]	[6.160, -0.003, 6.160, 6.160]
[5.0, -3.0, 7.0, 8.0]	0.003	0.1	[1.172, -0.703, 1.641, 1.876]	[5.005, -2.999, 6.995, 7.993]
[5.0, -3.0, 7.0, 8.0]	0.003	0.001	[0.118, -0.071, 0.165, 0.188]	[6.092, -0.932, 6.200, 6.267]
[5.0, -3.0, 7.0, 8.0]	0.003	1e-05	[0.012, -0.007, 0.017, 0.019]	[6.092, -0.932, 6.200, 6.267]
[-10.0, 4.0, 1.0, -5.0]	0.3	0.1	[-0.041, 0.016, 0.004, -0.020]	[-12.059, 6.070, 0.014, -6.139]
[-10.0, 4.0, 1.0, -5.0]	0.3	0.001	[-0.003, 0.001, 0.000, -0.001]	[-12.294, 6.152, 0.001, -6.158]
[-10.0, 4.0, 1.0, -5.0]	0.3	1e-05	[-0.000, 0.000, 0.000, -0.000]	[-12.315, 6.159, 0.000, -6.159]
[-10.0, 4.0, 1.0, -5.0]	0.003	0.1	[-2.388, 0.955, 0.239, -1.194]	[-10.002, 4.004, 0.995, -5.005]
[-10.0, 4.0, 1.0, -5.0]	0.003	0.001	[-0.240, 0.096, 0.024, -0.120]	[-11.748, 5.885, 0.063, -6.076]
[-10.0, 4.0, 1.0, -5.0]	0.003	1e-05	[-0.024, 0.010, 0.002, -0.012]	[-11.848, 5.938, 0.051, -6.092]
[1.0, -1.0, -3.0, 2.0]	0.3	0.1	[0.010, -0.010, -0.031, 0.020]	[0.007, -0.007, -0.314, 0.024]
[1.0, -1.0, -3.0, 2.0]	0.3	0.001	[0.001, -0.001, -0.002, 0.001]	[0.001, -0.001, -0.025, 0.002]
[1.0, -1.0, -3.0, 2.0]	0.3	1e-05	[0.000, -0.000, -0.000, 0.000]	[0.000, -0.000, -0.003, 0.000]
[1.0, -1.0, -3.0, 2.0]	0.003	0.1	[0.736, -0.736, -2.207, 1.471]	[0.995, -0.995, -2.999, 1.994]
[1.0, -1.0, -3.0, 2.0]	0.003	0.001	[0.073, -0.073, -0.220, 0.147]	[0.051, -0.051, -0.932, 0.143]
[1.0, -1.0, -3.0, 2.0]	0.003	1e-05	[0.007, -0.007, -0.022, 0.015]	[0.051, -0.051, -0.932, 0.143]

Table 2: Performance in gradient calculation for analytical and central difference approaches

x_i	function	$\nabla_{analytical}$	$\nabla_{approximate}$
[5.0, -3.0, 7.0, 8.0]	$f(x) = \sum_i^n x_i^2$	[10. -6. 14. 16.]	[10. -6. 14. 16.]
[5.0, -3.0, 7.0, 8.0]	$f(x) = \sum_i^n \frac{1}{100} x_i^2 - \cos(x)$	[-0.8589 -0.2011 0.797 1.1494]	[-0.8589 -0.2011 0.797 1.1494]
[-10. 4. 1. -5.]	$f(x) = \sum_i^n x_i^2$	[-20. 8. 2. -10.]	[-20. 8. 2. -10.]
[-10. 4. 1. -5.]	$f(x) = \sum_i^n \frac{1}{100} x_i^2 - \cos(x)$	[0.344 -0.6768 0.8615 0.8589]	[0.344 -0.6768 0.8615 0.8589]
[1. -1. -3. 2.]	$f(x) = \sum_i^n x_i^2$	[10. -6. 14. 16.]	[10. -6. 14. 16.]
[1. -1. -3. 2.]	$f(x) = \sum_i^n \frac{1}{100} x_i^2 - \cos(x)$	[0.8615 -0.8615 -0.2011 0.9493]	[0.8615 -0.8615 -0.2011 0.9493]

cost of performance as it'll take additional iterations to reach the higher level of precision. Here, we want to make sure that the convergence threshold isn't so small that we can never converge.

Unfortunately, it might not always be convenient to specify the gradient of our scalar function, $f(x)$, explicitly. This might be because it is complicated to compute, or because no closed form solution exists. In order to get around this issue, we can approximate the gradient of the function using central differences. We approximate the ith element of the gradient, ∇_i, as

$$\nabla_i \approx \frac{f(x_i + h) - f(x_i - h)}{2h} \tag{1}$$

where h is some small constant (we use $h = .001$).

We see that the performance in the calculation of the gradient is identical between the analytical approach and the central difference approach. That's great! Now let's see how our gradient descent algorithm compares to two more sophisticated optimizers - BFGS and Conjugate Gradient (CG). We compare both the number of iterations and function evaluations. We'll consider our algorithm in two forms - one where we pass in an explicit gradient function, and another where we estimate the gradient using the central difference method. All benchmarking is done with the same starting point: [5, -3, 7, 8]. $f_1(x) = \sum_i^n x_i^2$ and $f_2(x) = \sum_i^n x_i^{\frac{2}{100}} + \cos(x)$. We see that when passed an analytical solution for $\nabla f(x)$, our algorithm requires about as many function calls, although many more iterations than either BFGS or CG. If we use the central difference approximation for $\nabla f(x)$ instead, our algorithm requires many more iterations and function calls.

Table 3: Performance of authors' gradient descent algorithm compared to BFGS and CG

algorithm	$f_1(x)$ function calls	$f_1(x)$ iterations	$f_2(x)$ function calls	$f_2(x)$ iterations
BFGS	24	2	78	10
CG	30	2	78	6
Gradient Descent (analytical)	20	10	48	24
Gradient Descent (approximate)	100	10	240	24

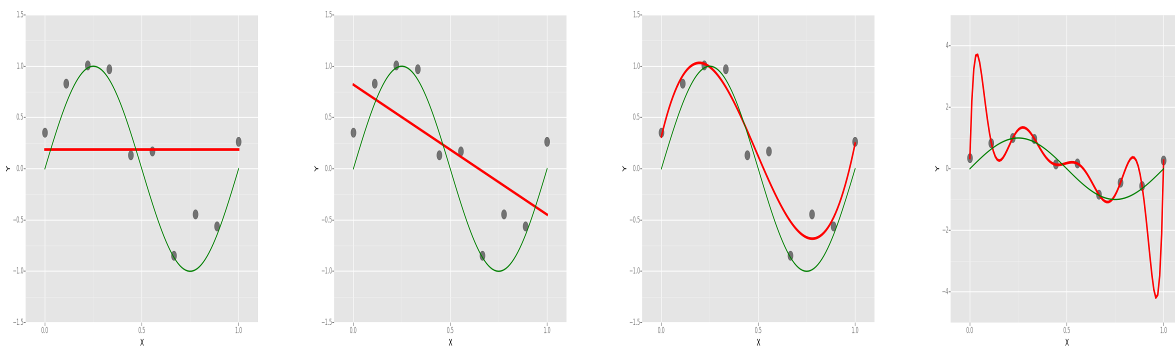
Problem 2

With problem 2, we first derive the maximum-likelihood estimator for the weight vector θ. Note that if we assume Gaussian errors, that is $Y \sim N(X\theta, \sigma^2)$, then our maximum-likelihood estimator is equivalent to the OLS estimator. Hence:

$$\hat{\theta}_{ML} = \hat{\theta}_{OLS} = (\Phi^T\Phi)^{-1}\Phi^T Y$$

where Φ denotes the polynomial basis expansion of X.

Using this closed form solution, we determined the maximum-likelihood weight vector for the polynomial basis expansions of X of orders 0, 1, 3, and 9. Using these estimated weight vectors we obtained very similar plots to Bishop as seen below:



$M = 0$ $M = 1$ $M = 3$ $M = 9$

Figure 1: Plots of polynomials having various orders M, in red, fitted to the the observed points. The green curve shows the DGF $\sin(2\pi x)$.

Table 4: Optimal Weight Vectors for Various Polynomial Basis Expansions of $\mathbf{X}$

	$M = 0$	$M = 1$	$M = 3$	$M = 9$
θ_0	0.186299	0.820212	0.313703	0.349482
θ_1		-1.267826	7.985371	232.682435
θ_2			-25.426102	-5329.068232
θ_3			17.374077	48633.377984
θ_4				-231944.259392
θ_5				640871.190655
θ_6				-1063154.903003
θ_7				1043711.192742
θ_8				-558375.328325
θ_9				125355.027159

The sum of squared errors of a linear polynomial basis model is defined by:

$$SSE = (\Phi\theta - Y)^T(\Phi\theta - Y)$$

which has gradient:

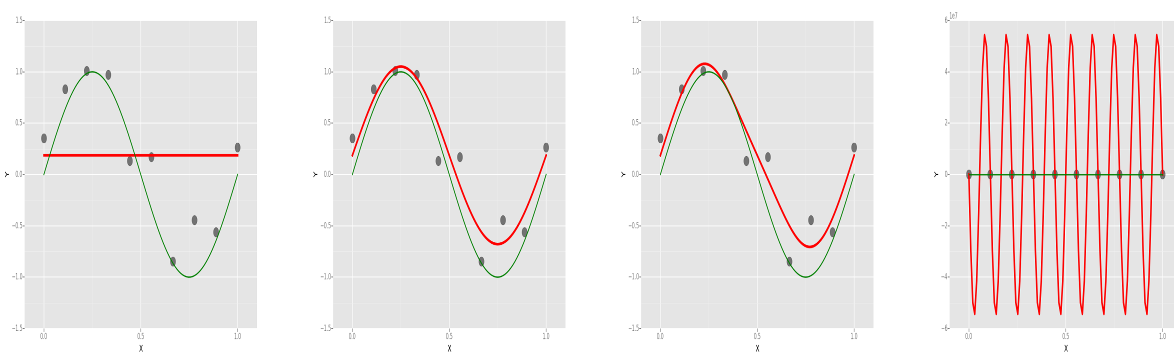
$$\nabla SSE = 2\Phi^T(\Phi\theta - Y)$$

We tested the accuracy to this closed form solution using our central differences approximator. The analytical and numerical gradients were essentially identical across many different points, even at order $M = 9$. This is exactly what we want!

We then applied gradient descent to the SSE function using the analytical gradient to see if we could replicate the plots in Bishop. Optimizing our hyperparameters got increasingly difficult as we increased the order M. For $M = O$, we merely needed to tune the step size and we could achieve consistent convergence to the Bishop plot across many different starting values. At $M = 1$, we needed to change both the step size and increase the number of maximum iterations before we consistently converged to the optimum. At $M = 3$, we also had to tune the convergence threshold to be several order of magnitudes smaller than it was before, and further increase the number of max interations to get consistent convergence. Finally $M = 9$, regardless of how we tried to tune the hyperparameters, we couldn't manage to find a set of hyperparameters that consistently converged, in fact, even scipy's BFGS optimizer failed to consistently produce a plot similar to Bishop's.

As we expected, our naive gradient descent implementation was vastly inferior the scipy's BFGS optimizer. While we could achieve the same level of accuracy as BFGS, our implementation took significantly more iterations. Furthermore, significant time and effort is needed to properly tune our algorithm's hyperparameters, while scipy's BFGS implementation didn't require any tuning.

Alternatively, we can use a trigonometric basis expansion rather than a polynomial one and get somewhat similar results. We expect that our SSE would converge to 0 as we increased the order M. Also, we expect the fit to the "true" data generating function would deteriorate again with increasing order M. This is in fact exactly what we see:



$M = 0$ $M = 1$ $M = 3$ $M = 9$

Figure 2: Plots of trigonometric basis expansions with various orders M, in red, fitted to the the observed points. The green curve shows the DGF $\sin(2\pi x)$.

Note that orders $M = 1$ and $M = 3$ provide rather good fits to for the true DGF. We should expect as the the DGF is in fact $\sin(2\pi x)$. However, if we didn't know that this was the true DGF, it might be problematic using a trigonometric basis expansion as it imposes a structure of cyclicality to the fit which may lead to gross misspecification of the model.

Problem 3

To begin problem 3, we implemented the closed form solution of Ridge Regression in Python, making use of Scipy and Numpy. Note that if you want to test cases where the number of features is greater than the number of data points (something that a well-trained teacher of machine should be skeptical to do), it is useful to use the pseudo-inverse, rather than the inverse to fit your parameters. We learned this the long way after debugging code for hours.

The closed form solution for ridge regression is given by the expression:

$$\hat{\theta} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^t\mathbf{y} \tag{2}$$

where $\mathbf{X}$ is your matrix of features, y is your array of observed values, and $\hat{\theta}$ are your estimated feature weights. λ is a regularization parameter, which represents how much you penalize the model for having large feature weights.

Given the data in Bishop 1.4 (which can be seen below), we attempt to fit polynomials of various orders, M.

Bishop_14_Data.png

The plot below shows the mean squared error (MSE) that our ridge regression fit gives for values of M between 1 and 5, for values of λ ranging from $10^0 - 1$ to 10^2. Note that in the case where $\lambda = 0$, we have OLS regression, and as M increases, the model is free to overfit our data. While the MSE here is low, if we evaluated this on a new data point, our model would likely perform very poorly. As λ gets higher, we penalize the model for adding additional large weights to $\hat{\theta}$, but our MSE stays relatively large. However, these "large" MSE models are likely to perform better on a new data point!

MSE_Lambda_Bishop.png

In order to avoid overfitting, but in order to make sure that we have chosen values of λ and M (and in general, hyperparameters) that make sense, it is common to split the data into a training set and a test set. We will use the closed-form solution for ridge regression to calculate $\hat{\theta}$ on our training set. We will then use that $\hat{\theta}$ to attempt to predict values of $\mathbf{y}$ for the test data. By choosing the $\hat{\theta}$ that minimizes MSE on the test data, but is trained on the training data, we are ensuring that we have not overfit our model to the data it is trained on. As one final step in the model selection process, we can check the performance of our final $\hat{\theta}$ on a validation set, to make sure that performance is still good (and we have not overfit for performance on our test set).

We use this methodology to find the best λ and M given three datasets similar to the bishop data. We calculate λ and M using the regress_train.txt, data we validate using regress_test.txt, and then we test using regress_validate.txt. We search through a grid of various values for λ and M, and find that MSE is lowest on the validation set when $\lambda = 1$ and $M = 1$: $MSE = 1.776$ on the validation data set. These parameters gave us an MSE of 1.460 on the training data and and an MSE of 1.415 on the test data. The fact that our MSE is on the same order of magnitude for the test data is a good sign - it indicates that in making sure we didn't overfit to the training data, we didn't accidentally overfit to the validation data.

The MSE for various combinations of λ and M on the three datasets (including our chosen set of hyperparameters) is found below. We see that with large M and small λ, we do great on the training data, but bad on our validation data. For large values of both λ and M, we do well, but not as well as our optimal values we found through the grid search.

Let's now use this methodology on a real dataset, as opposed to a toy dataset. The dataset that we will use was compiled by Kirsztian Buza at Budapest University of Technology and Economics. It includes 280 numerical values describing a number of blog posts, such as day of week, number of parent pages, and number of comments received within 24 hours. We are hoping to predict the number of comments it will receive in the next 24 hours. We are given this data split into training, validation, and test datasets, so we will once again perform a grid search to find the optimal value of λ. In this particular case, we are not regressing a polynomial of arbitrary order, so we do not need to test different values of M.

MSE_comparison.png

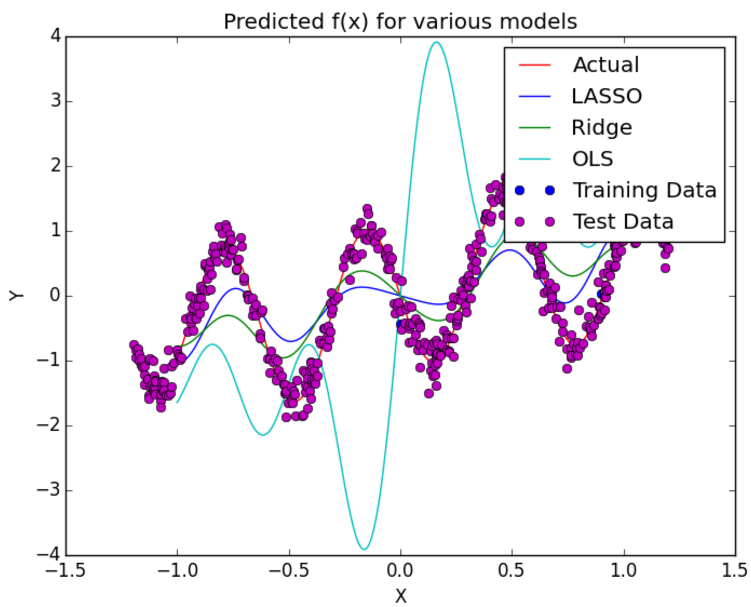
We find that for very large λ (as large as 10^6, MSE continues to decrease, although it is always close to 900. The MSE for a uniform predictor that predicts the average of y, $\hat{y}$, has an MSE of 1453, so the performance of our model is still better. However, we see that for values of λ higher than 10^6 or so, the value of the MSE increases, and eventually approaches (and eclipses) the MSE of our uniform estimator.

This isn't surprising - the blog feedback dataset is large, with 10,480 observations in the test set. If we interpret the value of λ as strength of our prior, it makes sense that it does not have a substantial effect until it is significantly larger than the size of our data. Furthermore, the inability of our model to get very low MSE for low λ speaks both to the fact that the data has a much higher dimension than our training data, and also suggests that the simple linear model we are using here may not be a very good fit for the data.

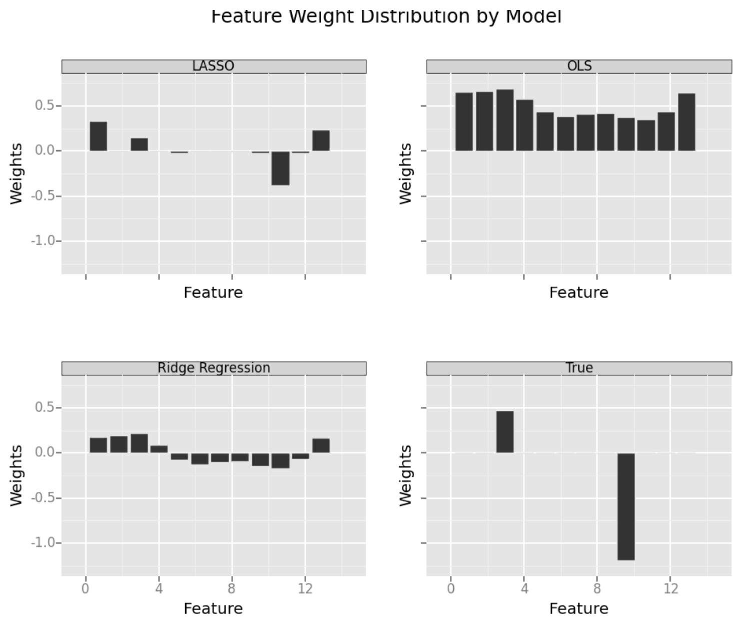
BlogFeedbackRegressionMSE.png

Problem 4

For problem 4, we are working with a highly sparse dataset so we can compare the differences between LASSO and ridge regression. We first start by determining the optimal penalty λ that minimizes the MSE of test set. Our optimal λ, 0.1, results in an MSE of 0.4395. When we disable the L_2 regularizer, our ridge regression produces the same estimated parameters as OLS which results in a MSE of 4.0979. Separately, we determine that $\lambda = .9$ is optimal LASSO penalty. This resulted in a MSE of 0.4524. We plotted our 3 obtained fits - OLS, Ridge with $\lambda = 0.1$, and LASSO with $\lambda = 0.9$ - against the the true DGF:



While its seems the ridge regression seems to fit the true DGF slightly better than LASSO, both these methods vastly outperform standard OLS. We further plotted the estimated optimal weight vectors from our 3 models against the true w:



We see that the L1 and L2 regularizers are working as intended! Our ridge regression estimates are considerably smaller than our OLS estimates. Furthermore, our we see sparse estimation from LASSO. This sparsity results from the differences between the L1 and L2 penalty. In ridge regression, we are want to minimize the squared error, subject to the constraint that the sum of the weights squared is less than some constant. Geometrically, we can think of this constraint as a sphere of some distance around the origin. In LASSO, we are minimizing the squared error subject to the constraint the the sum of the absolute values of the weights is less than some constant. The L1 constraint can be thought of as a diamond (or regular octahedral) around the origin.

Now consider sets weights that lead to the the same squared error. These sets which can represented as ellipses with the OLS estimates at their center, as that's the point the minimizes squared error. In Ridge regression, we are looking for the point where one of these ellipses touches the sphere around the origin, while in LASSO we're looking for the ellipse that touched the diamond. Since the diamond has shaper points, its fairly likely that the ellipse intersects the diamond at one of its points, we represents some weight begin equal to 0.