Homework 2: Ridge Regression and Gradient Descent

Name: Sujeong Cha / NetID: sjc433

```
In [1]: # import sys
   import numpy as np
   import pandas as pd
   import matplotlib.pyplot as plt
   from sklearn.model_selection import train_test_split
```

Computing Risk 1.(a)

$$E[x_i^2] = (0 * \frac{1}{5}) + (1 * \frac{2}{5}) + (4 * \frac{2}{5}) = 2$$

$$E[||x|||_2^2] = E[x_1^2 + \dots + x_n^2] = E[x_1^2] + \dots + E[x_n^2] = 2n$$

$$\therefore E[||x|||_2^2] = 2n$$

Computing Risk 1.(b)

When $E[\mid |x| \mid \infty] = 0$: every element should be zero $\rightarrow P(0) = (\frac{1}{5})^n$

When $E[\mid |x|\mid \infty]=1$: every element should be -1, 0, or 1 $\rightarrow P(1)=(\frac{3}{5})^n-(\frac{1}{5})^n$

When $E[\mid |x|\mid \infty]=2$: other than above cases $\rightarrow P(2)=1-(\frac{3}{5})^n$

$$E[\mid |x|\mid \infty] = (0*(\frac{1}{5})^n) + (1*((\frac{3}{5})^n - (\frac{1}{5})^n)) + (2*(1-(\frac{3}{5})^n))$$

$$\therefore E[||x|||\infty] = 2 - (\frac{1}{5})^n - (\frac{3}{5})^n$$

Computing Risk 1.(c)

$$\Sigma = \begin{pmatrix} 2 & 0 & \cdots & 0 \\ 0 & 2 & \cdots & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & \cdots & 2 \end{pmatrix}$$

The diagonal entries are variance of x_i which is equal to 2. $(Var(x_i) = E(x^2) - E(x)^2 = 2 - 0 = 2)$

The off-diagonal entries are all zero because x_i, x_j have covariance of zero (i.i.d. samples).

Computing Risk 2.(a)

$$E[(a-y)^2] = E[a^2 - 2ay + y^2] = E(a^2) - 2E(ay) + E(y^2) = a^2 - 2aE(y) + E(y^2)$$

Taking derivative on a and setting it equal to zero, 2a - 2E(y) = 0

$$\therefore a^* = E(y)$$

Substituting $a^* = E(y)$ to the expected loss, $E[(a^* - y)^2] = E(y)^2 - 2E(y)^2 + E(y^2) = E(y)^2 - 2E(y)^2 + Var(y) + E(y)^2$

$$\therefore E[(a^* - y)^2] = Var(y)$$

Computing Risk 2.(b).i

```
E[(a-y)^2|x] = E[a^2 - 2ay + y^2|x] = E[a^2|x] - E[2ay|x] + E[y^2|x] = a^2 - 2aE(y|x) + E(y^2|x)
Taking derivative on a and setting it equal to zero, 2a - 2E(y|x) = 0
\therefore a^* = f^*(x) = E(y|x)
```

Computing Risk 2.(b).ii

```
[Left Side]
```

```
\begin{split} &E[(f^*(x)-y)^2] = E[(E(y|x)-y)^2] = E[E(y|x)^2 - 2yE(y|x) + y^2] \\ &= E[E(y|x)E(y|x)] - 2E[yE(y|x)] + E[y^2] = E[E(y|x)]E[E(y|x)] - 2E[y]E[E(y|x)] + E[y^2] = E^2(y) - 2E^2(y) + E[y^2] = Var(y) \\ &\text{[Right Side]} \end{split}
```

The smallest value that the right side can take is Var(y) which is the Bayes risk found in 2.(a).

```
E[(f^*(x) - y)^2] \le E[(f(x) - y)^2]
```

Linear Regression 1.(a)

```
### Feature normalization
        def feature_normalization(train, test):
             ""Rescale the data so that each feature in the training set is in
           the interval [0,1], and apply the same transformations to the test
           set, using the statistics computed on the training set.
           Aras:
                train - training set, a 2D numpy array of size (num_instances, num_features)
               test - test set, a 2D numpy array of size (num_instances, num_features)
                train normalized - training set after normalization
                test_normalized - test set after normalization
            train_normalized = np.empty(train.shape)
            test_normalized = np.empty(test.shape)
            for i, column in enumerate(train.T):
               if max(column) == min(column):
                   train_normalized.T[i] = column
                   test_normalized.T[i] = test.T[i]
                else:
                   train_normalized_col = (column - min(column)) / (max(column) - min(column))
                   test_normalized_col = (test.T[i] - min(column)) / (max(column) - min(column))
                   train_normalized.T[i] = train_normalized_col
                   test_normalized.T[i] = test_normalized_col
            return train_normalized, test_normalized
```

Linear Regression 2.(a)

$$J(\theta) = \frac{1}{-}(X\theta - y)^{T}(X\theta - y)$$

Linear Regression 2.(b)

```
\nabla J(\theta) = \frac{2X^T X \theta - 2X^T y}{m}
```

Linear Regression 2.(c)

```
J(\theta + \eta h) - J(\theta) = \eta h^T \nabla J(\theta)
```

Linear Regression 2.(d)

```
\theta_i = \theta_{i-1} - \eta_{i-1} \nabla J(\theta_{i-1})
```

Linear Regression 2.(e)

Linear Regression 2.(f)

Linear Regression 3.(a)

```
### Gradient checker
        #Getting the gradient calculation correct is often the trickiest part
        #of any gradient-based optimization algorithm. Fortunately, it's very
        #easy to check that the gradient calculation is correct using the
        #definition of gradient.
        #See http://ufldl.stanford.edu/wiki/index.php/Gradient_checking_and_advanced_optimization
        def grad_checker(X, y, theta, epsilon=0.01, tolerance=1e-4):
              ""Implement Gradient Checker
            Check that the function compute_square_loss_gradient returns the
            correct gradient for the given X, y, and theta.
            Let d be the number of features. Here we numerically estimate the
            gradient by approximating the directional derivative in each of
            the d coordinate directions:
            (e_1 = (1,0,0,\ldots,0), e_2 = (0,1,0,\ldots,0), \ldots, e_d = (0,\ldots,0,1))
            The approximation for the directional derivative of J at the point
            theta in the direction e_i is given by:
            ( J(theta + epsilon * e_i) - J(theta - epsilon * e_i) ) / (2*epsilon).
            We then look at the Euclidean distance between the gradient
            computed using this approximation and the gradient computed by
            compute_square_loss_gradient(X, y, theta). If the Euclidean
            distance exceeds tolerance, we say the gradient is incorrect.
                X - the feature vector, 2D numpy array of size (num_instances, num_features)
                y - the label vector, 1D numpy array of size (num_instances)
                theta - the parameter vector, 1D numpy array of size (num_features)
                epsilon - the epsilon used in approximation
                tolerance - the tolerance error
            A boolean value indicating whether the gradient is correct or not
            true_gradient = compute_square_loss_gradient(X, y, theta) #The true gradient
            num features = theta.shape[0]
            approx_grad = np.zeros(num_features) #Initialize the gradient we approximate
            for i in range(num features):
                e = np.zeros(num_features)
                e[i] = 1
                d_i^i = (compute_square_loss(X, y, theta + epsilon * e) - compute_square_loss(X, y, theta - epsilon * e)) / (2 *
        epsilon)
                approx_grad[i] = d_i
            return np.linalg.norm(true gradient-approx grad) < tolerance</pre>
```

Linear Regression 4.(a)

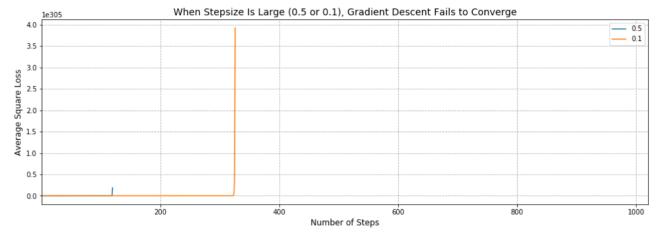
```
### Batch gradient descent
        def batch grad descent(X, y, alpha=0.1, num step=1000, grad check=False):
            In this question you will implement batch gradient descent to
            minimize the average square loss objective.
               X - the feature vector, 2D numpy array of size (num_instances, num_features)
                y - the label vector, 1D numpy array of size (num_instances)
               alpha - step size in gradient descent
               num_step - number of steps to run
               grad_check - a boolean value indicating whether checking the gradient when updating
                theta_hist - the history of parameter vector, 2D numpy array of size (num_step+1, num_features)
                            for instance, theta in step 0 should be theta_hist[0], theta in step (num_step) is theta_hist[-1]
                loss_hist - the history of average square loss on the data, 1D numpy array, (num_step+1)
            num_instances, num_features = X.shape[0], X.shape[1]
            theta_hist = np.zeros((num_step+1, num_features)) #Initialize theta_hist
            loss hist = np.zeros(num step+1) #Initialize loss hist
            theta = np.zeros(num_features) #Initialize theta
            for i in range(1, num_step+1):
                theta = theta - alpha * compute_square_loss_gradient(X, y, theta)
                if grad_check == True:
                   if grad_checker(X, y, theta) == False: raise ValueError('Wrong Gradient')
                loss = compute_square_loss(X, y, theta)
                theta hist[i] = theta
                loss_hist[i] = loss
            return theta_hist, loss_hist
```

Linear Regression 4.(b)

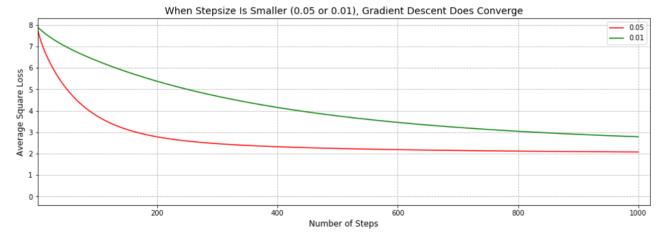
```
In [7]: | df = pd.read_csv('ridge_regression_dataset.csv', delimiter=',')
        X = df.values[:,:-1]
        y = df.values[:,-1]
        print('Split into Train and Test')
        X_train, X_test, y_train, y_test = train_test_split(X, y, test_size =100, random_state=10)
        print("Scaling all to [0, 1]")
        X train, X test = feature normalization(X train, X test)
        X_train = np.hstack((X_train, np.ones((X_train.shape[0], 1)))) # Add bias term
        X_test = np.hstack((X_test, np.ones((X_test.shape[0], 1)))) # Add bias term
        Split into Train and Test
        Scaling all to [0, 1]
In [8]: stepsize = [0.5, 0.1, 0.05, 0.01]
        losses = np.empty((4, 1001))
        for i, s in enumerate(stepsize):
            th, lh = batch_grad_descent(X_train, y_train, alpha = s)
            losses[i] = lh
```

C:\Users\sujeong\Anaconda3\lib\site-packages\ipykernel_launcher.py:15: RuntimeWarning: overflow encountered in multiply from ipykernel import kernelapp as app

```
In [9]: plt.figure(figsize=(16,5))
    plt.grid('gray', linestyle = '--')
    plt.plot(losses[0])
    plt.plot(losses[1])
    plt.legend(stepsize, loc='upper right')
    plt.xlim(1, 1020)
    plt.xlabel("Number of Steps", fontsize=12)
    plt.ylabel("Average Square Loss", fontsize=12)
    plt.title("When Stepsize Is Large (0.5 or 0.1), Gradient Descent Fails to Converge", fontsize=14)
    plt.show()
```



```
In [10]: plt.figure(figsize=(16,5))
    plt.grid('gray', linestyle = '--')
    plt.plot(losses[2], c='red')
    plt.plot(losses[3], c='green')
    plt.legend(stepsize[2:], loc='upper right')
    plt.xlim(1, 1020)
    plt.xlabel("Number of Steps", fontsize=12)
    plt.ylabel("Average Square Loss", fontsize=12)
    plt.title("When Stepsize Is Smaller (0.05 or 0.01), Gradient Descent Does Converge", fontsize=14)
    plt.show()
```



When we choose stepsize to be too large (i.e. 0.5 or 0.1), the gradient descent might fail to converge (Top Graph). On the other hand, if we decrease the stepsize (i.e. 0.05 or 0.01), the gradient descent does converge (Bottom Graph). Thus, it is crucial to choose an appropriate stepsize.

Ridge Regression 1

$$\nabla J(\theta) = \frac{2X^T X \theta - 2X^T y}{m} + 2\lambda \theta$$

$$\theta_i = \theta_{i-1} - \eta_{i-1} \nabla J(\theta_{i-1})$$

Ridge Regression 2

Ridge Regression 3

```
### Regularized batch gradient descent
         def regularized_grad_descent(X, y, alpha=0.05, lambda_reg=10**-2, num_step=1000):
             Aras:
                X - the feature vector, 2D numpy array of size (num_instances, num_features)
                y - the label vector, 1D numpy array of size (num_instances)
                alpha - step size in gradient descent
                 lambda reg - the regularization coefficient
                num_step - number of steps to run
                theta hist - the history of parameter vector, 2D numpy array of size (num step+1, num features)
                             for instance, theta in step 0 should be theta_hist[0], theta in step (num_step+1) is theta_hist[-
         1]
                 loss hist - the history of average square loss function without the regularization term, 1D numpy array.
             num instances, num features = X.shape[0], X.shape[1]
             theta = np.zeros(num_features) #Initialize theta
             theta_hist = np.zeros((num_step+1, num_features)) #Initialize theta_hist
             loss_hist = np.zeros(num_step+1) #Initialize loss_hist
             for i in range(1, num_step+1):
                 theta = theta - alpha * compute_regularized_square_loss_gradient(X, y, theta, lambda_reg)
                 loss = compute_square_loss(X, y, theta)
                 theta hist[i] = theta
                 loss_hist[i] = loss
             return theta_hist, loss_hist
```

Ridge Regression 4

If we make the bias term B arbitrarily large (say, 100000) compared to the actual intercept value (10), the weight coefficient for the bias term will be very small (10^{-4}). Thus, the penalizing parameter λ does not have much effect on the weight coefficient for the bias term, resulting in weak regularization.

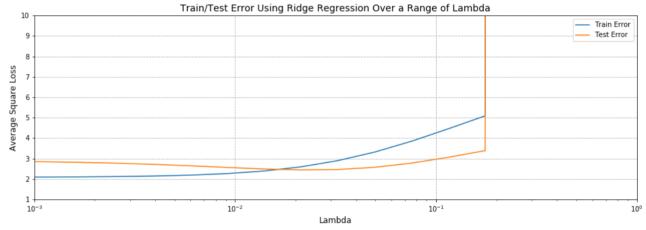
Ridge Regression 5

```
In [13]: lambda_search = np.logspace(-7, 2)
lambda_losses_train = []
lambda_losses_test = []
last_theta = []

for lamb_ in lambda_search:
    th, lh = regularized_grad_descent(X_train, y_train, lambda_reg=lamb_)
    last_theta.append(th[-1])
    lambda_losses_train.append(lh[-1])
    lambda_losses_train.append(compute_square_loss(X_test, y_test, th[-1]))
C:\Users\sujeong\Anaconda3\lib\site-packages\ipykernel_launcher.py:16: RuntimeWarning: overflow encountered in multiply app.launch_new_instance()
```

C:\Users\sujeong\Anaconda3\lib\site-packages\ipykernel_launcher.py:23: RuntimeWarning: invalid value encountered in sub tract

```
In [14]: plt.figure(figsize=(16,5))
    plt.grid('gray', linestyle = '--')
    plt.semilogx(lambda_search, lambda_losses_train)
    plt.semilogx(lambda_search, lambda_losses_test)
    plt.xlim(10**-3, 10**0)
    plt.ylim(1, 10)
    plt.legend(['Train Error', 'Test Error'])
    plt.xlabel("Lambda", fontsize=12)
    plt.ylabel("Average Square Loss", fontsize=12)
    plt.title("Train/Test Error Using Ridge Regression Over a Range of Lambda", fontsize=14)
    plt.show()
```



Ridge Regression 6

In practice, I would use **RandomizedSearchCV** function in scikit-learn to find the optimal combination of parameter (lambda, stepsize, etc) and the corresponding theta. We could also use GirdSearchCV but it can be time-wise inefficient because it searches through every possible combination of parameters. Instead, RandomizedSearchCV checks for only parts of the combinations, reducing the computing time albeit not producing the lowest-possible error.

Stochastic Gradient Descent 1

$$f_i(\theta) = (h_{\theta}(x_i) - y_i)^2 + \lambda \theta^T \theta$$

Stochastic Gradient Descent 2

$$E[\nabla f_i(\theta)] = \frac{1}{m} \sum_{i=1}^m \nabla f_i(\theta) = \nabla \frac{1}{m} \sum_{i=1}^m f_i(\theta) = \nabla J(\theta)$$

Stochastic Gradient Descent 3

$$\theta_i = \theta_{i-1} - \eta_{i-1} \nabla f_{i-1}(\theta)$$

Stochastic Gradient Descent 4

```
### Stochastic gradient descent
         def stochastic_grad_descent(X, y, alpha=0.01, lambda_reg=10**-2, num_epoch=1000, alpha_type='fixed'):
             In this question you will implement stochastic gradient descent with regularization term
                 X - the feature vector, 2D numpy array of size (num_instances, num_features)
                 y - the label vector, 1D numpy array of size (num_instances)
                 alpha - string or float, step size in gradient descent
                         NOTE: In SGD, it's not a good idea to use a fixed step size. Usually it's set to 1/sqrt(t) or 1/t
                         if alpha is a float, then the step size in every step is the float.
                         if alpha == "1/sqrt(t)", alpha = 1/sqrt(t).
                         if alpha == "1/t", alpha = 1/t.
                 lambda_reg - the regularization coefficient
                 num_epoch - number of epochs to go through the whole training set
                 theta_hist - the history of parameter vector, 3D numpy array of size (num_epoch, num_instances, num_features)
                             for instance, theta in epoch 0 should be theta_hist[0], theta in epoch (num_epoch) is theta_hist[-
         1]
                loss hist - the history of loss function vector, 2D numpy array of size (num_epoch, num_instances)
             num instances, num_features = X.shape[0], X.shape[1]
             theta = np.ones(num_features) #Initialize theta
             theta_hist = np.zeros((num_epoch, num_instances, num_features)) #Initialize theta_hist
             loss_hist = np.zeros((num_epoch, num_instances)) #Initialize loss_hist
             C=alpha
             for e in range(num_epoch):
                 s = np.arange(num_instances)
                 np.random.shuffle(s)
                 for i in s:
                     X_{\underline{}} = X[i]
                     y_{-} = y[i]
                     if alpha_type == 'fixed': alpha_ = C
                     if alpha_type == 'C/t': alpha_ = C / t
                     if alpha_type == 'C/sqrt(t)': alpha_ = C / np.sqrt(t)
                     theta = theta - alpha_ * compute_regularized_square_loss_gradient(X_, y_, theta, lambda_reg)
                     loss = compute_square_loss(X, y, theta)
                     theta_hist[e][i] = theta
                     loss_hist[e][i] = loss
                     t += 1
             return theta_hist, loss_hist
```

Stochastic Gradient Descent 5

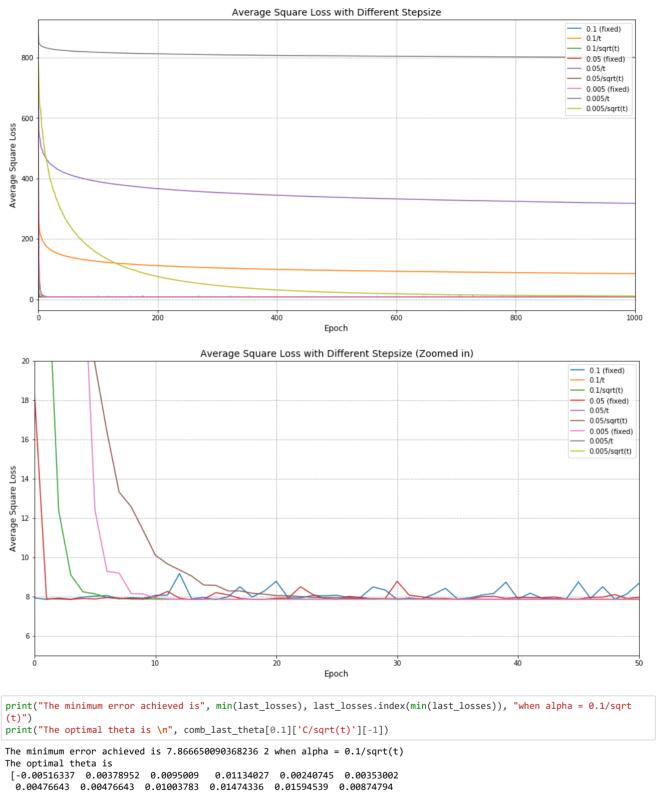
```
In [30]: step_size = [0.1, 0.05, 0.005]
step_type = ['fixed', 'C/t', 'C/sqrt(t)']

comb_last_theta = {}
comb_losses_train = {}
last_losses = []

for size in step_size:
    losses_train = {}
    last_theta = {}
    for steptype in step_type:
        th, lh = stochastic_grad_descent(X_train, y_train, alpha = size, lambda_reg=10**-2, num_epoch=1000, alpha_type=steptype)

    last_theta[steptype] = th[:,-1]
    losses_train[steptype] = lh[:,-1]
    last_losses.append(lh[-1, -1])
    comb_last_theta[size] = last_theta
    comb_losses_train[size] = losses_train
```

```
In [19]: plt.figure(figsize=(16, 8))
         plt.grid('gray', linestyle = '--')
         plt.plot(comb_losses_train[0.1]['fixed'])
plt.plot(comb_losses_train[0.1]['C/t'])
         plt.plot(comb_losses_train[0.1]['C/sqrt(t)'])
         plt.plot(comb_losses_train[0.05]['fixed'])
plt.plot(comb_losses_train[0.05]['C/t'])
         plt.plot(comb_losses_train[0.05]['C/sqrt(t)'])
         plt.plot(comb_losses_train[0.005]['fixed'])
         plt.plot(comb_losses_train[0.005]['C/t'])
         plt.plot(comb_losses_train[0.005]['C/sqrt(t)'])
        plt.xlabel("Epoch", fontsize=12)
         plt.ylabel("Average Square Loss", fontsize=12)
         plt.xlim(0, 1000)
         plt.title("Average Square Loss with Different Stepsize", fontsize=14)
         plt.show()
         plt.figure(figsize=(16, 8))
         plt.grid('gray', linestyle = '--')
         plt.plot(comb_losses_train[0.1]['fixed'])
         plt.plot(comb_losses_train[0.1]['C/t'])
         plt.plot(comb_losses_train[0.1]['C/sqrt(t)'])
         plt.plot(comb_losses_train[0.05]['fixed'])
         plt.plot(comb_losses_train[0.05]['C/t'])
         plt.plot(comb_losses_train[0.05]['C/sqrt(t)'])
         plt.plot(comb_losses_train[0.005]['fixed'])
         plt.plot(comb_losses_train[0.005]['C/t'])
         plt.plot(comb_losses_train[0.005]['C/sqrt(t)'])
        plt.xlabel("Epoch", fontsize=12)
         plt.ylabel("Average Square Loss", fontsize=12)
         plt.xlim(0, 50)
         plt.ylim(5, 20)
         plt.title("Average Square Loss with Different Stepsize (Zoomed in)", fontsize=14)
         plt.show()
```



```
In [40]: print("The minimum error achieved is", min(last_losses), last_losses.index(min(last_losses)), "when alpha = 0.1/sqrt
           0.00047624 -0.00416237
                                  0.01385354
                                             0.01608134
                                                         0.01300753
                                                                     0.0026437
           0.00410118 0.00410118 0.00410118
                                              0.00574409
                                                         0.00574409
                                                                     0.00574409
           0.00604756 0.00604756 0.00604756
                                              0.006183
                                                         0.006183
                                                                     0.006183
           0.00625653
                      0.00625653
                                  0.00625653
                                              0.0067115
                                                         0.0067115
                                                                     0.0067115
           0.00755184 0.00755184 0.00755184 0.00708634 0.00708634 0.00708634
           0.00686674 0.00686674 0.00686674 0.00674361 0.00674361 0.00674361
          -0.00780978]
```

As the first graph shows, the loss function did not converge when stepsize was 'C/t' regardless of the value of C. Interestingly, the fixed step size of 0.05 converged to the possible minimum fastest. Fixed step size of 0.1 also converged to the minimum very fast but it tends to fluctuate in the later epoch due to the larger step size. The best step size might differ depending on the shape of the objective function, but for our loss function, fixed step sizes performed better than other non-constant step sizes.

In []:	