## ML hw2

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# 1 Gradescope

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# 2 Computing Risk

# 2.1 Expectations

1(a) 
$$E[||\vec{x}||_2^2] = E[x_1^2 + ... + x_n^2] = nE[x_i^2] = n((-2)^2 + (-1)^2 + 0^2 + 1^2 + 2^2)/5 = 2n$$
  
1(b)  $E[||\vec{x}||_{\infty}] = E[max_i|x_i|] = (-2)/5 + 2/5 = 4/5$   
1(c) For the elements in  $\Sigma_{\vec{x}}$ ,  $\Sigma_{ii} = Var[x_i] = E[x_i^2] - E[x_i]^2 = 2$ ,  $\Sigma_{ij} = 0$  ( $i \neq j$ )

### 2.2 Bayes risk

2(a) We have 
$$E[a] = a$$
,  $Var[a] = 0$   
 $E[(a - y)^2] = E[a^2 + y^2 - 2ay] = E[a^2] + E[y^2] - 2E[ay] = Var(a) + E[a]^2 + Var(y) + E[y]^2 - 2aE[y] = Var[y] + (a - E[y])^2$   
Therefore,  $a^* = E[y]$ , the Bayes risk is  $Var[y]$ 

### 2.3 Bayes decision function

2(b)(i)

We have 
$$E[a|x]=a$$
,  $Var[a|x]=0$ , because a is a deterministic function of x.  $E[(a-y)^2|x]=E[a^2+y^2-2ay|x]=E[a^2|x]+E[y^2|x]-2E[ay|x]=Var(a|x)+E[a|x]^2+Var(y|x)+E[y|x]^2-2aE[y|x]=Var[y|x]+(a-E[y|x])^2$  Therefore,  $a^*=E[y|x]$ , the Bayes risk is  $Var[y|x]$ 

2(b)(ii)

$$E[(f^*(x) - y)^2] = E[E[(f^*(x) - y)^2 | x]] \le E[E[(f(x) - y)^2 | x]] = E[(f(x) - y)^2]$$

The first and the second equality uses the law of iterated expectations. The inequality uses the given fact that  $E[(f^*(x) - y)^2 | x] \le E[(f(x) - y)^2 | x]$ , Since the expectations are scaler, so the inequality of the expectations of these expectations is also true.

# 3 Linear Regression

### 3.1 Feature normalization

1(a)

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

```
### 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.
        Args:
             train - training set, a 2D numpy array of size (num_instances, \Box
      \hookrightarrow num_features)
             test - test set, a 2D numpy array of size (num_instances, num_features)
        Returns:
             train_normalized - training set after normalization
             test_normalized - test set after normalization
        train_min = np.amin(train, axis=0)
        train_max = np.amax(train, axis=0)
        train_range = train_max - train_min
        del_li = []
        for i in range(len(train_range)):
            if train_range[i] == 0:
                del_li.append(i)
        train = np.delete(train, del_li, axis=1)
        test = np.delete(test, del_li, axis=1)
        train_range = np.delete(train_range, del_li)
        train_min = np.delete(train_min, del_li)
        train_normalized = (train - train_min) / train_range
        test_normalized = (test - train_min) / train_range
        return train_normalized, test_normalized
```

loading the dataset Split into Train and Test Scaling all to [0, 1]

### 3.2 Objective function

2(a) 
$$J = \frac{1}{m} \sum_{i=1}^{m} (\theta^T x_i - y_i)^2 = \frac{1}{m} |X\theta - Y|^2 = \frac{1}{m} (X\theta - Y)^T (X\theta - Y)$$

### 3.3 Gradient of objective function

$$2(b) \nabla J = \frac{2}{m} X^T (X\theta - Y)$$

# 3.4 Using first order approximation

2(c) 
$$J(\theta + \eta h) \simeq J(\theta) + \eta h^T \nabla J(\theta)$$

### 3.5 Update expression

$$2(d) \theta' = \theta - \eta \nabla I(\theta)$$

### 3.6 Compute square loss

2(e)

```
Args:
    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 array of size (num_features)

Returns:
    loss - the average square loss, scalar
"""

loss = 0 #Initialize the average square loss
#TODO

m = X.shape[0]
diff = np.dot(X, theta) - y
loss = 1/(2*m) * np.dot(diff, diff)
return loss
```

### 3.7 Compute square loss gradient

2(f)

```
### The gradient of the square loss function
     def compute_square_loss_gradient(X, y, theta):
         Compute the gradient of the average square loss (as defined in_{\sqcup}
      \rightarrow compute_square_loss), at the point theta.
        Args:
            X - the feature vector, 2D numpy array of size (num_instances, _
      \rightarrow num_features)
            y - the label vector, 1D numpy array of size (num_instances)
             theta - the parameter vector, 1D numpy array of size (num_features)
        Returns:
             grad - gradient vector, 1D numpy array of size (num_features)
        #TODO
        m = X.shape[0]
        diff = np.dot(X, theta) - y
        grad = (1/m) * np.dot(diff, X)
        return grad
```

#### 3.8 Gradient checker

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/
      \rightarrow 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, \dots, 0), e_2 = (0, 1, 0, \dots, 0), \dots, e_d = (0, \dots, 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.
         Args:
             \it X - the feature vector, 2D numpy array of size (num_instances, \it \square
       \rightarrow 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
         Return:
             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
         #TODO
         for i in range(num_features):
             e_i = np.zeros(num_features)
             ei[i] = 1
             approx_grad[i] = 1/(2*epsilon) *_
```

```
compute_square_loss(X,y,(theta-epsilon*e_i)))
return np.linalg.norm(true_gradient - approx_grad) < tolerance</pre>
```

```
### Generic gradient checker
     def generic_gradient_checker(X, y, theta, objective_func, gradient_func,_
       ⇒epsilon=0.01, tolerance=1e-4):
          11 11 11
          The functions takes objective_func and gradient_func as parameters.
         And check whether gradient_func(X, y, theta) returned the true
         gradient for objective_func(X, y, theta).
         Eq: In LSR, the objective_func = compute_square_loss, and qradient_func = \Box
       ⇒compute_square_loss_gradient
          11 11 11
         #T∩D∩
         true_gradient = gradient_func(X, y, theta) #The true gradient
         num_features = theta.shape[0]
         approx_grad = np.zeros(num_features) #Initialize the gradient we approximate
         #TODO
         for i in range(num_features):
             e_i = np.zeros(num_features)
             e_i[i] = 1
             approx_grad[i] = 1/(2*epsilon) *_
       →(objective_func(X,y,(theta+epsilon*e_i)) -
                                        objective_func(X,y,(theta-epsilon*e_i)))
           print(true_gradient, approx_grad)
         return np.linalg.norm(true_gradient - approx_grad) < tolerance
```

#### 3.9 Batch gradient descent

4(a) (Taking all examples as a batch)

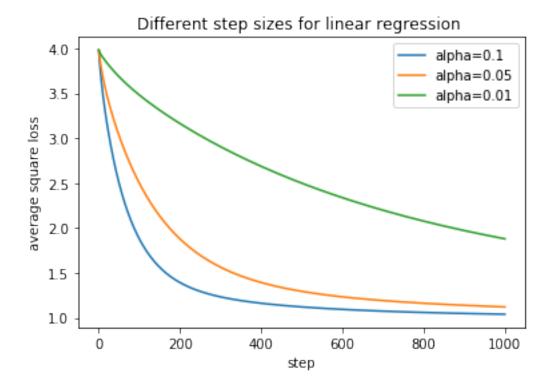
```
Returns:
       theta\_hist - the history of parameter vector, 2D numpy array of size_{\sqcup}
→ (num_step+1, num_features)
                    for instance, theta in step 0 should be theta_hist[0], __
\rightarrow theta in step (num_step) is theta_hist[-1]
       loss_hist - the history of average square loss on the data, 1D numpy_{\sqcup}
\rightarrow 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
   #TODO
  grad_err = False
  theta_hist[0] = theta
  for i in range(num_step):
       loss = compute_square_loss(X, y, theta)
       loss_hist[i] = loss
       grad = compute_square_loss_gradient(X, y, theta)
       if grad_check and grad_checker(X,y,theta) == False:
           print("alpha=",alpha,"grad error at step", i)
           grad_err = True
           break
       theta = theta - alpha * grad
       theta_hist[i+1] = theta
  loss_hist[i+1] = compute_square_loss(X, y, theta)
  return theta_hist, loss_hist, grad_err
```

#### 3.10 Experiment on step size

alpha= 0.4 grad error at step 7

4(b)

alpha= 0.3 grad error at step 9 alpha= 0.2 grad error at step 12



Conclusion: When alpha(step size)=0.1, 0.05, 0.01, the average square loss converges, and it converges faster when alpha is larger. However, when alpha grows larger, e.g. alpha=0.2,0.3,0.4,0.5, the average square loss does not converge.

# 4 Ridge Regression

## 4.1 Vector gradient of J

$$\nabla J(\theta) = \frac{2}{m} X^{T} (X\theta - Y) + 2\lambda \theta^{T}$$
  
Updating  $\theta$ :  $\theta' = \theta - \eta \nabla J(\theta)$ 

### 4.2 Compute regularized square loss gradient

### 4.3 Regularized gradient descent

```
### Regularized batch gradient descent
      def regularized_grad_descent(X, y, alpha=0.05, lambda_reg=10**-2, num_step=1000,__
       →grad_check=False):
          11 11 11
          Args:
              X - the feature vector, 2D numpy array of size (num_instances, ⊔
       \rightarrow num_features)
              y - the label vector, 1D numpy array of size (num_instances)
              alpha - step size in gradient descent
              lambda_req - the regularization coefficient
              num_step - number of steps to run
          Returns:
              theta_hist - the history of parameter vector, 2D numpy array of size_{\sqcup}
       \rightarrow (num_step+1, num_features)
                           for instance, theta in step 0 should be theta_hist[0], _
       \rightarrow 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
          #TODO
          grad_err = False
          theta_hist[0] = theta
          for i in range(num_step):
              loss = compute_square_loss(X, y, theta)
              loss_hist[i] = loss
```

```
grad = compute_regularized_square_loss_gradient(X, y, theta, lambda_reg)
if grad_check and grad_checker(X,y,theta) == False:
    print("alpha=",alpha,"grad error at step", i)
    grad_err = True
    break
theta = theta - alpha * grad
theta_hist[i+1] = theta
loss_hist[i+1] = compute_square_loss(X, y, theta)
return theta_hist, loss_hist, grad_err
```

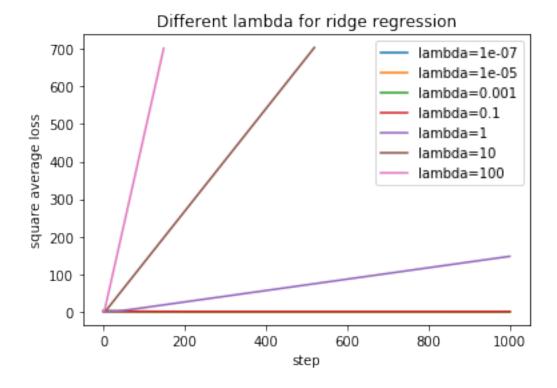
### 4.4 Explain bias in optimization

The bias term is the product of B and the last column in theta. When applying a regularization, if B is very large, the adjustment on theta would be small. Therefore, the effectiveness of regularization on bias term is decreased. We could set B approching infinity to make the regularization negligible.

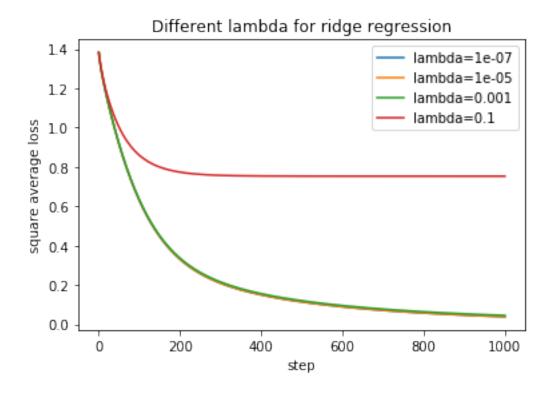
### 4.5 Find optimal parameter

Find the lambda that minimize the average square loss (without regularization part) on the test set. First we fix B=1, set step size (alpha) to 0.1 (which is the optimal alpha from the previous experiments) and try a range of lambda.

```
[28]: plt_lambda_reg([1e-7,1e-5,1e-3,1e-1,1, 10,100])
```



When lambda=1, 10 or 100, the loss diverges.

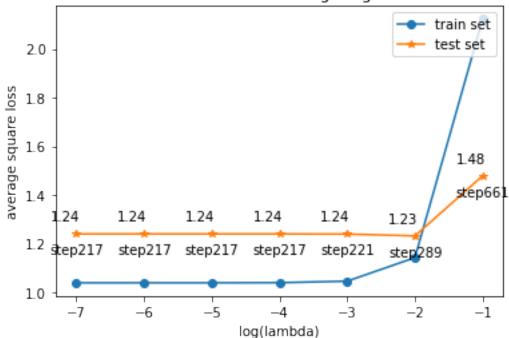


When lambda=0.1,0.001,1e-5,1e-7, the loss converges.

In order to find the lambda with the minimal loss on test set, we compare the minimal loss among all steps for different lambda.

```
[66]: a = 0.1
      # TODO: choose alpha from backtracking line search
      li = [1e-7, 1e-6, 1e-5, 1e-4, 1e-3, 1e-2, 1e-1]
      train_loss = []
      test_loss = []
      steps = []
      for l in li:
          # train loss
          theta_hist, loss_hist, grad_err = regularized_grad_descent(X_train,y_train,u
       →alpha=a, lambda_reg=1, num_step=1000)
          train_loss.append(loss_hist[-1])
          # test loss
          test_loss_hist= [compute_square_loss(X_test,y_test,theta) for theta in_
       →theta_hist]
          # find the minimum test loss with theta from all training steps
            test_loss.append(test_loss_hist[-1])
          i = np.argsort(test_loss_hist)[0]
          test_loss.append(test_loss_hist[i])
          steps.append(i)
```





We choose labmda=0.01 as the optimal lambda, since test loss reaches the minimum.

#### 4.6 What theta to select

In practice, choose the theta when using lambda=0.01 and step=289, because it achieves the minimum loss on test set.

### 5 Stochastic Gradient Descent

### 5.1 Objective function equivalence

$$f_{i}(\theta) = (h_{\theta}(x_{i}) - y_{i})^{2} + \lambda \theta^{T} \theta$$

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} f_{i}(\theta) = \frac{1}{m} \sum_{i=1}^{m} ((h_{\theta}(x_{i}) - y_{i})^{2} + \lambda \theta^{T} \theta) = \frac{1}{m} \sum_{i=1}^{m} (h_{\theta}(x_{i}) - y_{i})^{2} + \lambda \theta^{T} \theta$$

#### 5.2 Prove unbiased estimator

```
Left of the equation: E[\nabla f_i(\theta)] = \sum_{i=1}^m P(i) \nabla f_i(\theta) = \sum_{i=1}^m \frac{1}{m} \nabla f_i(\theta)
Right of the equation: \nabla J(\theta) = \nabla (\frac{1}{m} \sum_{i=1}^m f_i(\theta)) = \frac{1}{m} \sum_{i=1}^m \nabla f_i(\theta)
Therefore, E[\nabla f_i(\theta)] = \nabla J(\theta)
```

### 5.3 Update rule

 $\theta' = \theta - stepsize * \nabla f_i(\theta)$  for every sample  $x_i$ 

### 5.4 Implement SGD

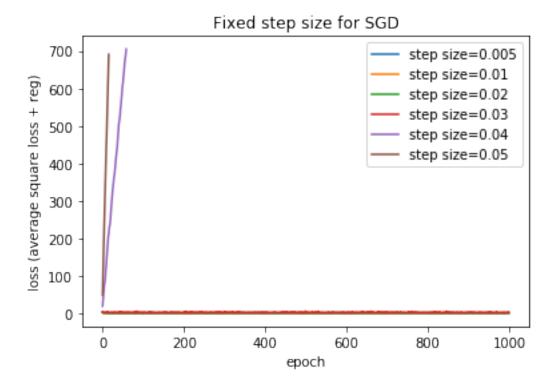
```
if alpha is a float, then the step size in every step is the
 \hookrightarrow float.
                if \ alpha == "1/sqrt(t)", \ alpha = 1/sqrt(t).
                if alpha == "1/t", alpha = 1/t.
        lambda_reg - the regularization coefficient
        num_epoch - number of epochs to go through the whole training set
    Returns:
        theta\_hist - the history of parameter vector, 3D numpy array of size_{\sqcup}
 → (num_epoch, num_instances, num_features)
                      for instance, theta in epoch 0 should be theta_hist[0], _
 \hookrightarrow theta in epoch (num_epoch) is theta_hist[-1]
        loss hist - the history of loss function vector, 2D numpy array of size\Box
 → (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_
 \rightarrow theta_hist
    loss_hist = np.zeros((num_epoch, num_instances)) #Initialize loss_hist
    #TODO
    for i in range(num_epoch):
        # shuffle
        idx = np.arange(num_instances)
        random.shuffle(idx)
        X = X[idx]
        y = y[idx]
        loss = 0
        for j in range(num_instances):
            if alpha == '1/sqrt(t)':
                alpha = c/np.sqrt((i*num_epoch+j+1))
            elif alpha == '1/t':
                alpha = c/(i*num_epoch+j+1)
            theta_hist[i][j] = theta
            diff = np.dot(X[j],theta) - y[j]
            loss = np.dot(diff,diff) + lambda_reg * np.dot(theta,theta)
            loss_hist[i][j] = loss
            grad = 2*(np.dot(diff,X[j])+lambda_reg*theta)
            theta = theta - alpha * grad
          if i%100==0:
#
              print('epoch=',i,'loss=',np.mean(loss_hist[i],axis=0))
    return theta_hist, loss_hist
```

### 5.5 Find optimal parameters

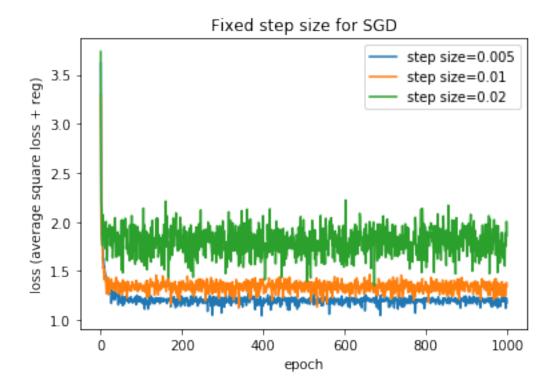
(1) Fixed step size

```
[78]: plt_fix_sgd([0.005,0.01,0.02,0.03,0.04,0.05])
```

/opt/conda/envs/dsga-1003/lib/python3.7/site-packages/ipykernel\_launcher.py:48: RuntimeWarning: overflow encountered in multiply



```
[79]: plt_fix_sgd([0.005,0.01,0.02])
```

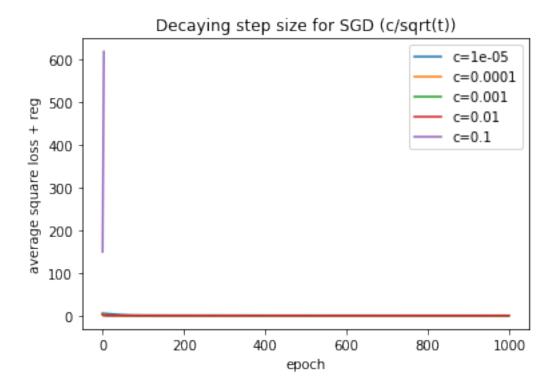


### (2) Decaying step size using different schedules

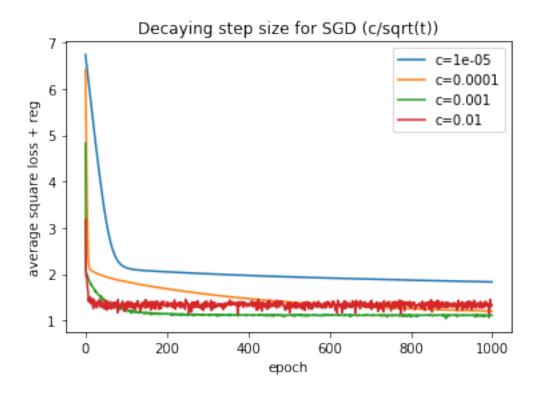
```
[29]: def plt_decay_sgd(li, alpha):
    for c in li:
        theta_hist, loss_hist = stochastic_grad_descent(X_train, y_train, u)
        alpha=alpha, c=c)
        avg_loss_hist = np.mean(loss_hist, axis=1)
        plt.plot(range(len(avg_loss_hist)),np.
        →log(avg_loss_hist),label="c="+str(c))
        plt.title('Decaying step size for SGD (c'+ alpha[1:] + ')')
        plt.xlabel("epoch")
        plt.ylabel("average square loss + reg")
        plt.legend(loc = 1)
        plt.show()
```

```
[30]: plt_decay_sgd([1e-5, 1e-4, 1e-3, 1e-2, 0.1], '1/sqrt(t)')
```

/opt/conda/envs/dsga-1003/lib/python3.7/site-packages/ipykernel\_launcher.py:51: RuntimeWarning: overflow encountered in multiply

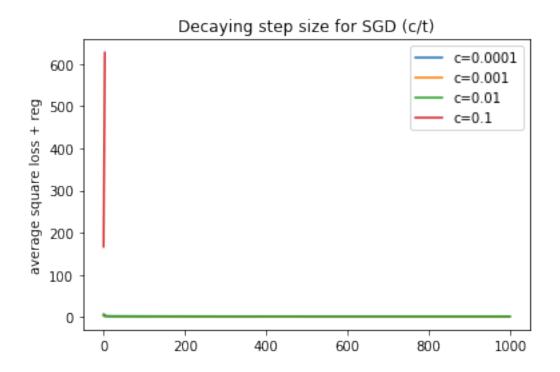


When the initial step size c=0.1, it is too aggressive that the loss function does not converge.

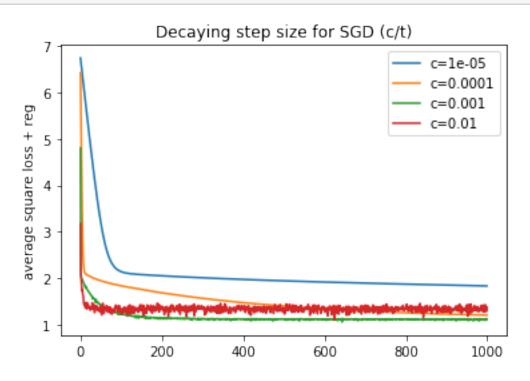


The when c<0.001, the loss function converges too slow. When c>0.001, it does not reach the minimum loss. So the best configuration is c=0.001 for the schema  $step \ size = c/sqrt(t)$ .

/opt/conda/envs/dsga-1003/lib/python3.7/site-packages/ipykernel\_launcher.py:48: RuntimeWarning: overflow encountered in multiply



When the initial step size c=0.1, it is too aggressive that the loss function does not converge.



The when c<0.001, the loss function converges too slow. When c>0.001, it does not reach the minimum loss. So the best configuration is c=0.001 for the schema  $step \ size = c/t$ .

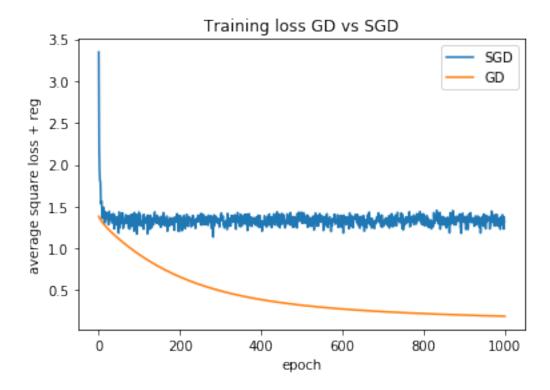
### (3) Compare GD with SGD

```
[94]: import time
    start_time = time.time()
    theta_hist, loss_hist = stochastic_grad_descent(X_train, y_train)
    print('SGD training time for 1000 epoch',time.time()-start_time)
    avg_loss_hist = np.mean(loss_hist, axis=1)
    plt.plot(range(len(avg_loss_hist)),np.log(avg_loss_hist),label='SGD')

    start_time = time.time()
    theta_hist, loss_hist, _ = regularized_grad_descent(X_train, y_train)
    print('GD training time for 1000 epoch',time.time()-start_time)
    plt.plot(range(len(loss_hist)),np.log(loss_hist),label='GD')

    plt.title('Training loss GD vs SGD')
    plt.xlabel("epoch")
    plt.ylabel("average square loss + reg")
    plt.legend(loc = 1)
    plt.show()
```

SGD training time for 1000 epoch 1.841592788696289 GD training time for 1000 epoch 0.02275848388671875



It shows that SDG converges slower than GD once we get close to the minimizer.

## 5.6 Adaptive step size

(1) average theta

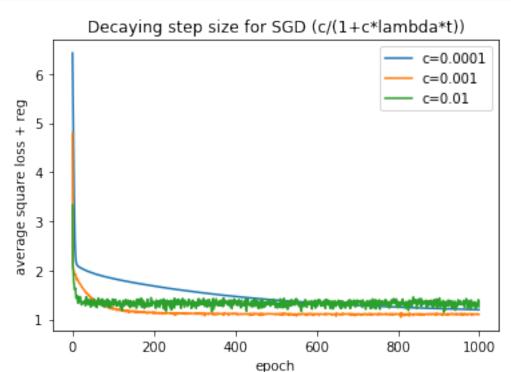
test loss with last step theta: 4.0259 test loss with average theta: 3.285

(2) The new stepsize rule:  $stepsize = \frac{c}{1+c\lambda t}$ 

```
### Stochastic gradient descent
      import random
      def stochastic_grad_descent(X, y, alpha=0.01, lambda_reg=10**-2, num_epoch=1000,__
       \rightarrowc=0.1):
          In this question you will implement stochastic gradient descent with \sqcup
       \rightarrow regularization term
          Args:
              X - the feature vector, 2D numpy array of size (num_instances, \Box
       \rightarrow 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.
       \rightarrow 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 \Box
       \hookrightarrow float.
                       if \ alpha == "1/sqrt(t)", \ alpha = 1/sqrt(t).
```

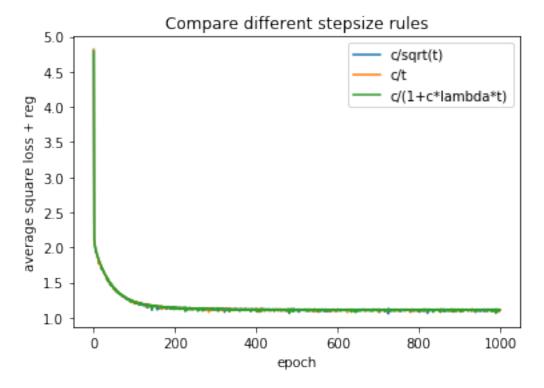
```
if alpha == "1/t", alpha = 1/t.
       lambda_req - the regularization coefficient
       num_epoch - number of epochs to go through the whole training set
  Returns:
       theta\_hist - the history of parameter vector, 3D numpy array of size_{\sqcup}
→ (num_epoch, num_instances, num_features)
                    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_{\sqcup}
→ (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_
\rightarrow theta_hist
  loss_hist = np.zeros((num_epoch, num_instances)) #Initialize loss_hist
  #TODO
  for i in range(num_epoch):
       # shuffle
       idx = np.arange(num_instances)
      random.shuffle(idx)
      X = X[idx]
       y = y[idx]
       loss = 0
       for j in range(num_instances):
           t = i*num_epoch+j+1
           if alpha == '1/sqrt(t)':
               alpha = c/np.sqrt(t)
           elif alpha == '1/t':
               alpha = c/t
           elif alpha == 'new':
               alpha = c/(1+c*lambda_reg*t)
           theta_hist[i][j] = theta
           diff = np.dot(X[j],theta) - y[j]
           loss = np.dot(diff,diff) + lambda_reg * np.dot(theta,theta)
           loss_hist[i][j] = loss
           grad = 2*(np.dot(diff,X[j])+lambda_reg*theta)
           theta = theta - alpha * grad
  return theta_hist, loss_hist
```

(i) Find the best parameter *c* 



When  $\eta_0 = 0.001$ , the loss function converges with the minimum.

(ii) Compare different stepsize rules with their optimal parameters



The three stepsize rules have similar performances.