Lab: Nonlinear Least Squares for Modeling Materials

Nonlinear least squares (NLLS) is a widely-used method for modeling data. In NLLS, we wish to fit a model of the form,

```
yhat = g(x,w)
```

where `w` is a vector of paramters and `x` is the vector of predictors. We find `w` by minimizing a least-squares function

```
f(w) = \sum_i (y_i - g(x_i,w))^2
```

where the summation is over training samples `(x_i,y_i)`. This is similar to linear least-squares, but the function `g(x,w)` may not be linear in `w`. In general, this optimization has no closed-form expression. So numerical optimization must be used.

In this lab, we will implement gradient descent on NLLS in a problem of physical modeling of materials. Specifically, we will estimate parameters for expansion of copper as a function of temperature using a real dataset. In doing this lab, you will learn to:

- Set up a nonlinear least squares as an unconstrained optimization function
- Compute initial parameter estimates for a simple rational model
- Compute the gradients of the least squares objective
- Implement gradient descent for minimizing the objective
- Implement momentum gradient descent
- Visualize the convergence of the algorithm

We first import some key packages.

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from sklearn.linear_model import Ridge, LinearRegression
```

Load the Data

The NIST agency has an excellent nonlinear regression website that has several datasets for nonlinear regression problems. In this lab, we will use the data from a NIST study involving the thermal expansion of copper. The response variable is the coefficient of thermal expansion, and the predictor variable is temperature in degrees kelvin.

> Hahn, T., NIST (1979), Copper Thermal Expansion Study. (unpublished}

You can download the data as follows.

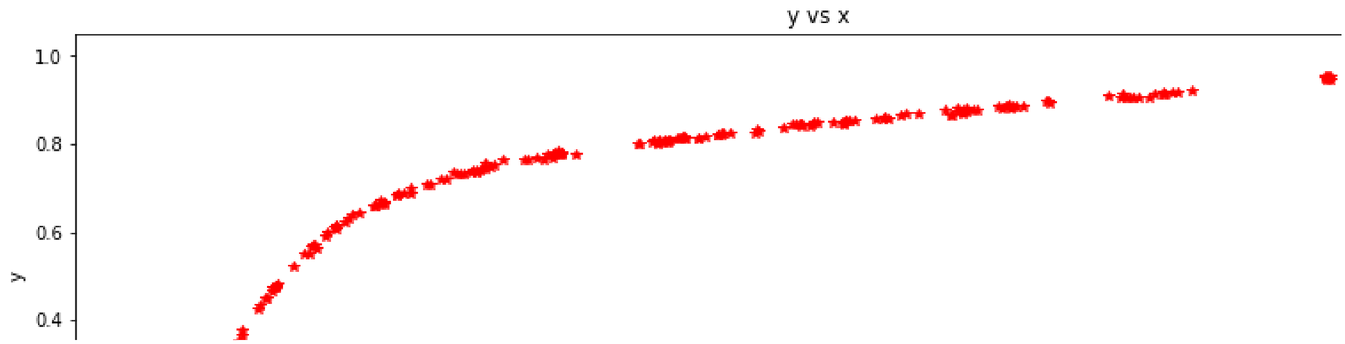
```
url = 'https://itl.nist.gov/div898/strd/nls/data/LINKS/DATA/Hahn1.dat'
df = pd.read_csv(url, skiprows=60, sep=' ',skipinitialspace=True, names=['y0','x0','dummy'])
df.head()
```

	y0	x0	dummy
0	0.591	24.41	NaN
1	1.547	34.82	NaN
2	2.902	44.09	NaN
3	2.894	45.07	NaN
4	4.703	54.98	NaN

Extract the `x0` and `y0` into arrays. Rescale, `x0` and `y0` to values between `0` and `1` by dividing `x0` and `y0` by the maximum value. Store the scaled values in vectors `x` and `y`. The rescaling will help with the conditioning of the fitting. Plot, `y` vs. `x`.

```
# TODO
x0 = df['x0']
y0 = df['y0']
x = x0/np.max(x0)
y = y0/np.max(y0)
args = np.argsort(x)
x = x[args]
y = y[args]
x = np.asarray(x)
y = np.asarray(y)
plt.figure(figsize=(15,5))
plt.plot(x,y,'*r')
plt.xlabel('x')
plt.ylabel('y')
plt.title('y vs x')
```

```
Text(0.5, 1.0, 'y vs x')
```

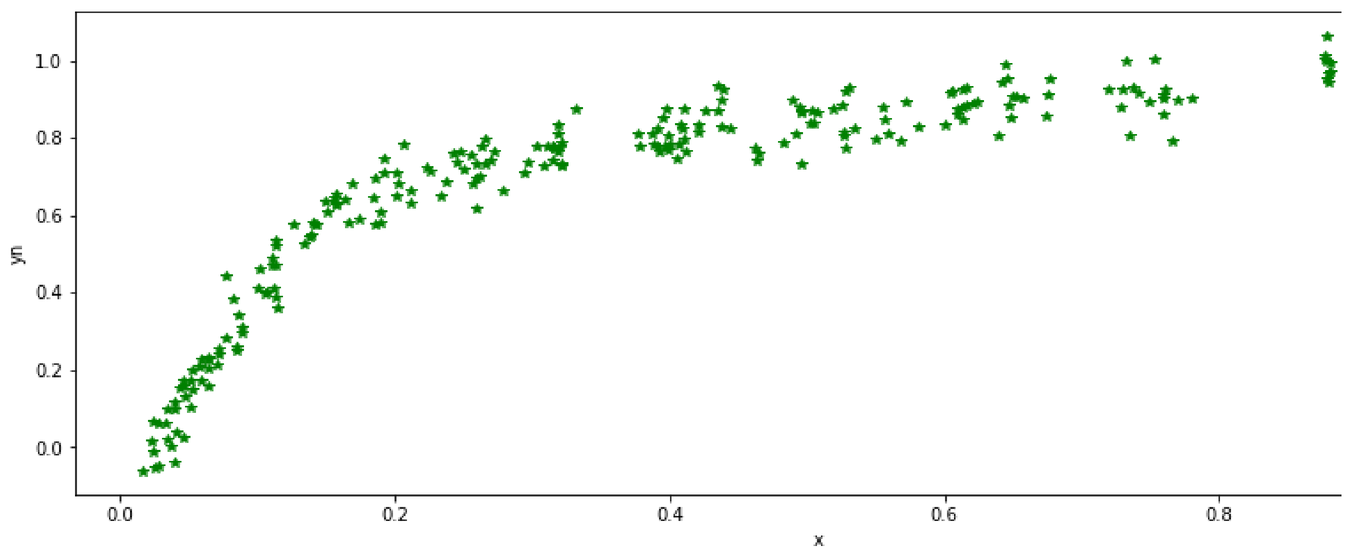


To make the problem a little more challenging, we will add some noise. Add random Gaussian noise with mean 0 and std. dev = 0.02 to `y`. Store the noisy results in `yn`. You can use the `np.random.normal()` function to add Gaussian noise. Plot `yn` vs. `x`.

0.0 0.2 0.4 0.6 0.8

```
# TODO
mu, sigma = 0, 0.05 # mean and standard deviation
yn = y + np.random.normal(mu,sigma,size=y.shape)
plt.figure(figsize=(15,5))
plt.plot(x,yn,'*g')
plt.xlabel('x')
plt.ylabel('yn')#
```

```
Text(0, 0.5, 'yn')
```



Split the data `(x,yn)` into training and test. Let `xtr,ytr` be training data and `xts,yts` be the test data. You can use the `train_test_split` function. Set `test_size=0.33` so that 1/3 of the samples are held out for test.

```
from sklearn.model_selection import train_test_split
```

```
# TODO
xtr, xts, ytr, yts = train_test_split(x, yn,test_size= 0.33,shuffle= True)
print(xtr.shape)
```

```
(158,)
```

Initial Fit for a Rational Model

The [NIST website](#) suggests using a *rational* model of the form,

```
yhat = (a[0] + a[1]*x + ... + a[d]*x^d)/(1 + b[0]*x + ... + b[d-1]*x^d)
```

with `d=3`. The model parameters are `w = [a[0],...,a[d],b[0],...,b[d-1]]` so there are `2d+1` parameters total. Complete the function below that takes vectors `w` and `x` and predicts a set of values `yhat` using the above model.

```
def predict(w,x):

  # Get the length
  d = (len(w)-1)//2
  # TODO. Extract a and b from w
  a = w[0: d+1]
  b = w[d+1:]
  # But, remember you must flip the order the a and b
  a=np.flip(a)
  b = np.concatenate(([1],b))
  b=np.flip(b)
  # TODO. Compute yhat. You may use the np.polyval function
  yhat_a = np.polyval(a,x)
  yhat_b= np.polyval(b,x)
  yhat=yhat_a/yhat_b
  return yhat
```

When we fit with a nonlinear model, most methods only get convergence to a local minima. So, you need a good initial condition. For a rational model, one way to get is to realize that if:

```
y ~= (a[0] + a[1]*x + ... + a[d]*x^d)/(1 + b[0]*x + ... + b[d-1]*x^d)
```

Then:

```
y ~= a[0] + a[1]*x + ... + a[d]*x^d - b[0]*x*y + ... - b[d-1]*x^d*y.
```

So, we can solve for the the parameters `w = [a,b]` from linear regression of the predictors,

```
Z[i,:] = [ x[i], ... , x[i]**d, y[i]*x[i], ... , y[i}*x[i]**d ]
```

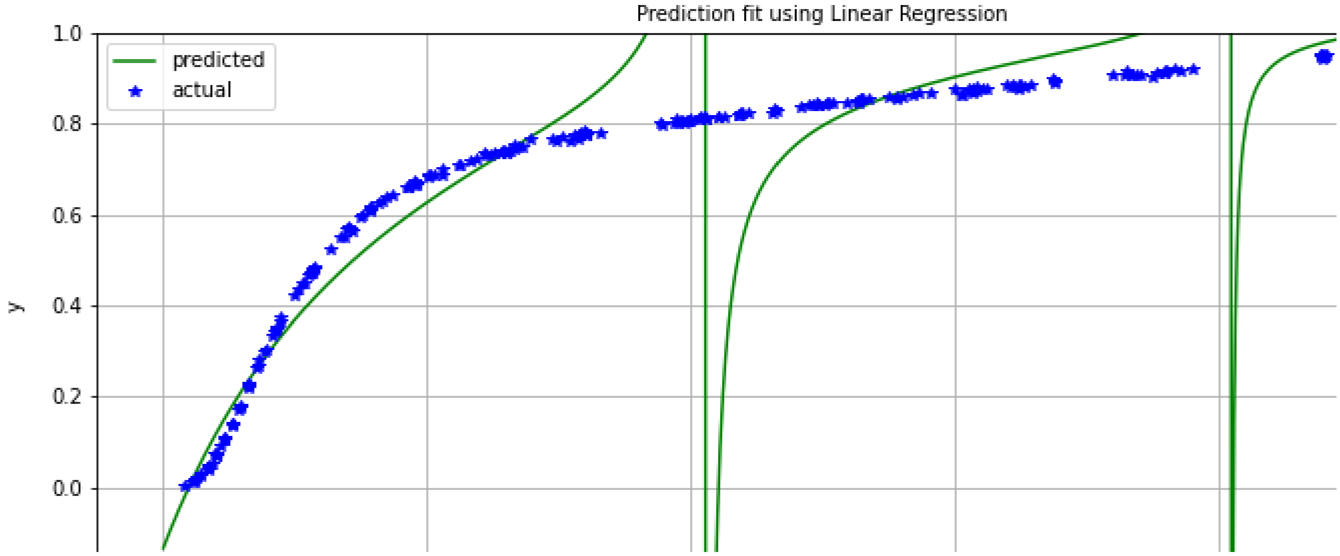
```
d = 3
dp=np.arange(1,d+1)
print(dp)
Z = np.zeros((len(xtr),2*d))
#print(Z)
for i in range(len(xtr)):
    k= np.power(xtr[i],dp)
    #print(k)
    l= ytr[i]*np.power(xtr[i],dp)
    #print(l)
    Z[i,:] = np.concatenate((k,l))
model = LinearRegression()
model.fit(Z,ytr)
# TODO
a = np.concatenate(([model.intercept_],model.coef_[0:d]))
b = -model.coef_[d:]
winit = np.concatenate((a,b))
```

```
[1 2 3]
```

Now plot the predicted values of the `yhat` vs. `x` using your estimated parameter `winit` for 1000 values `x` in `[0,1]`. On the same plot, plot `yts` vs. `xts`. You will see that you get a horrible fit.

```
# TODO
xp = np.linspace(0,1,num=1000)
yhat = np.zeros(len(xp))
for i in range(len(xp)):
    yhat[i] = predict(winit,xp[i])
i = np.argsort(xts)
xts, yts = xts[i], yts[i]
plt.figure(figsize=(13,5))
plt.plot(xp,yhat,'g')
plt.plot(x,y,'*b')
plt.xlabel('x')
plt.ylabel('y')
plt.legend(('predicted','actual'),fontsize=10)
plt.title('Prediction fit using Linear Regression',fontsize=10)
plt.grid()
plt.ylim([-0.2,1])
```

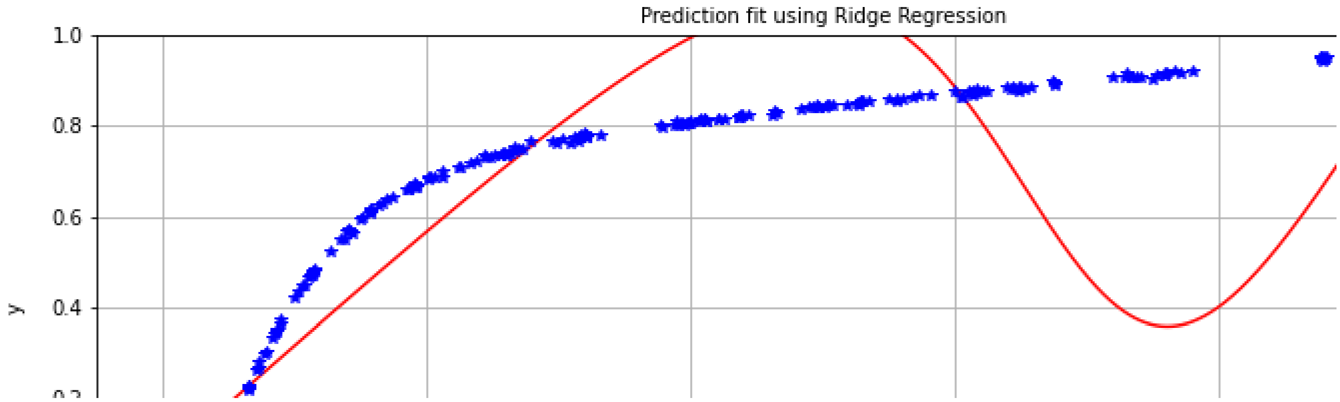
```
(-0.2, 1.0)
```



The reason the previous fit is poor is that the denominator in `yhat` goes close to zero. To avoid this problem, we can use Ridge regression, to try to keep the parameters close to zero. Re-run the fit above with `Ridge` with `alpha = 1e-3`. You should see you get a reasonable, but not perfect fit.

```
# TODO.  Fit with parameters with linear regression
reg = Ridge(alpha=1e-3)
reg.fit(Z,ytr)
# TODO
# Extract the parameters from regr.coef_ and regr.intercept_
a = np.concatenate(([reg.intercept_],reg.coef_[0:d]))
b = -reg.coef_[d:]
winit = np.concatenate((a,b))
# TODO
# Plot the results as above.
xp = np.linspace(0,1,num=1000)
yhat = np.zeros(len(xp))
yhat[:] = predict(winit,xp[:])
plt.figure(figsize=(13,5))
plt.plot(xp,yhat,'r')
plt.plot(x,y,'*b')
plt.xlabel('x')
plt.ylabel('y')
plt.title('Prediction fit using Ridge Regression',fontsize=10)
plt.grid()
plt.ylim([-0.2,1])
```

```
(-0.2, 1.0)
```



Creating a Loss Function

We can now use gradient descent to improve our initial estimate. Complete the following function to compute

```
f(w) = 0.5*\sum_i (y[i] - yhat[i])^2
```

and `fgrad`, the gradient of `f(w)`.

```
def feval(w,x,y):
    d = (len(w)-1)//2
    a = w[0:d+1]
    b = w[d+1:]
    # TODO. Znum[i,j] = x[i]**j
    Znum = np.zeros((len(x),d+1))
    for i in range(len(x)):
        for j in range(d+1):
            Znum[i,j] = x[i]**j
        # TODO. Zden[i,j] = x[i]**(j+1)
        Zden = np.zeros((len(x),d))
    for i in range(len(x)):
        for j in range(d):
            Zden[i,j] = x[i]**(j+1)
    yhat = np.zeros(len(x))

    for i in range(len(x)):
        yhat[i] = Znum[i,:].dot(a)/(1+Zden[i,:].dot(b))

    f = 0.5*np.sum(np.square(y-yhat))

    grada = np.zeros(len(a))

    for j in range(len(a)):
        grada[j] = -np.sum((y-yhat)*Znum[:,j]/(1+np.matmul(Zden,b)))
    gradb = np.zeros(len(b))
```

```
    for j in range(len(b)):
        gradb[j] = np.sum((y-yhat)*yhat*Zden[:,j]/(1+np.matmul(Zden,b)))

    fgrad = np.concatenate((grada,gradb))
    return f, fgrad
```

Test the gradient function:

- Take `w0=winit` and compute `f0,fgrad0 = feval(w0,xtr,ytr)`
- Take `w1` very close to `w0` and compute `f1,fgrad1 = feval(w1,xtr,ytr)`
- Verify that `f1-f0` is close to the predicted value based on the gradient.

```
# TODO
w0 = winit
f0, fgrad0 = feval(w0,xtr,ytr)
w1 = w0 + 1e-6
f1,fgrad1 = feval(w1,xtr,ytr)
print('Actual Difference: %.4f'%(f1-f0))
print('Predicted Difference using gradient: %.4f'%(fgrad0.dot(w1-w0)))
```

```
Actual Difference: -0.0002
Predicted Difference using gradient: -0.0002
```

Implement gradient descent

We will now try to minimize the loss function with gradient descent. Using the function `feval` defined above, implement gradient descent. Run gradient descent with a step size of `alpha=1e-6` starting at `w=winit`. Run it for `nit=10000` iterations. Compute `fgd[it]` = the objective function on iteration `it`. Plot `fgd[it]` vs. `it`.

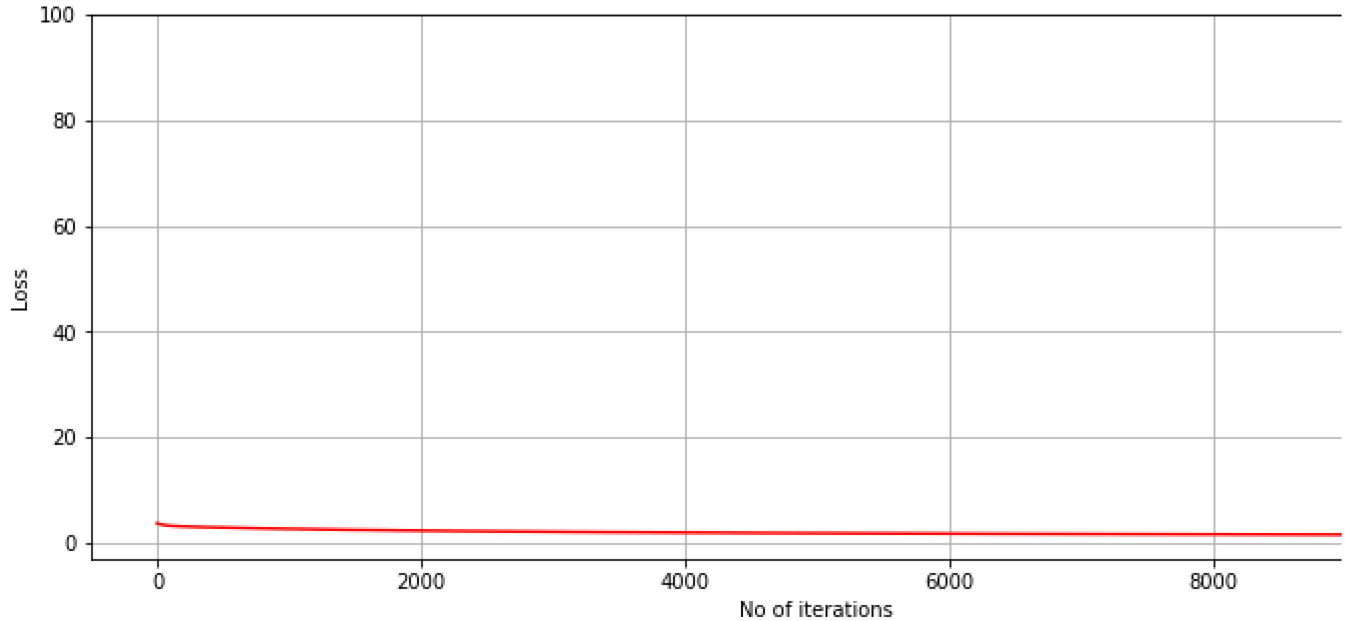
You should see that the training loss decreases, but it still hasn't converged after 10000 iterations.

```
# TODO
# fgd = ...
nit = 10000
step = 1e-6
# Create history dictionary for tracking progress per iteration.
# This isn't necessary if you just want the final answer, but it
# is useful for debugging
hist = {'w': [], 'f': []}
for i in range(nit):
    f0, fgrad0 = feval(w0,xtr,ytr)
    w0 = w0 - fgrad0*step
    hist['w'].append(w0)
    hist['f'].append(f0)
```

```
for elem in ('f', 'w'):
    hist[elem] = np.array(hist[elem])

t = np.arange(nit)
loss = np.array(hist['f'])
plt.figure(figsize=(13,5))
plt.plot(t,loss,'r-')
plt.xlabel('No of iterations')
plt.ylabel('Loss')
plt.grid()
plt.ylim(-3,100)
```

```
(-3.0, 100.0)
```



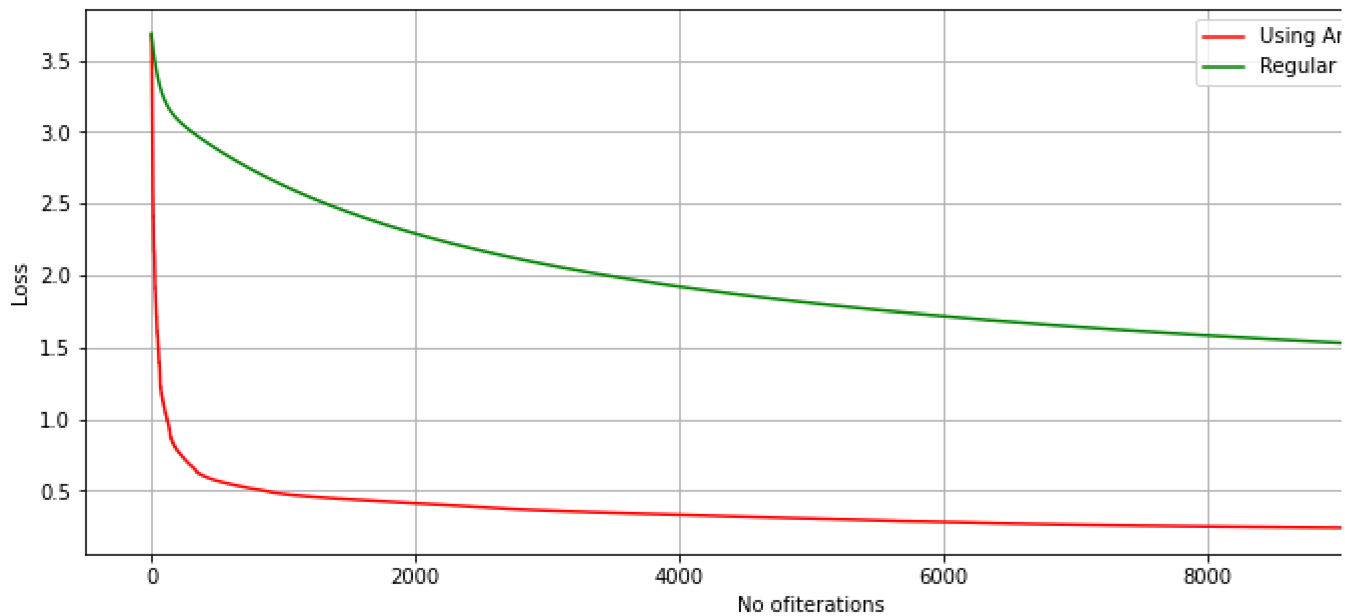
Now, try to get a faster convergence with adaptive step-size using the Armijo rule. Implement the gradient descent with adaptive step size. Let `fadapt[it]` be the loss function on iteration `it`. Plot `fadapt[it]` and `fgd[it]` vs. `it` on the same graph. You should see a slight improvement, but not much.

```
# TODO
# fadapt = ...
nit = 10000
step = 1e-6 # Initial step
hist = {'w':[],'f':[]}
w0 = winit; f0, fgrad0 = feval(winit,xtr,ytr)
for i in range(nit):
    w1 = w0 - fgrad0*step
    f1, fgrad1 = feval(w1,xtr,ytr)
    df = fgrad0.dot(w1-w0)
    al = 0.5
    if (f1-f0 < al*df) and (f1<f0):
```

```
            step = step*2
            f0 = f1
            fgrad0 = fgrad1
            w0 = w1
        else:
            step = step/2
        hist['w'].append(w0)
        hist['f'].append(f0)

loss_arm = np.array(hist['f'])
plt.figure(figsize=(13,5))
plt.plot(loss_arm,'r-')
plt.plot(loss,'g-')
plt.xlabel('No ofiterations')
plt.ylabel('Loss')
plt.grid()
plt.legend(('Using Armijo Rule','Regular Gradient Descent'))
```

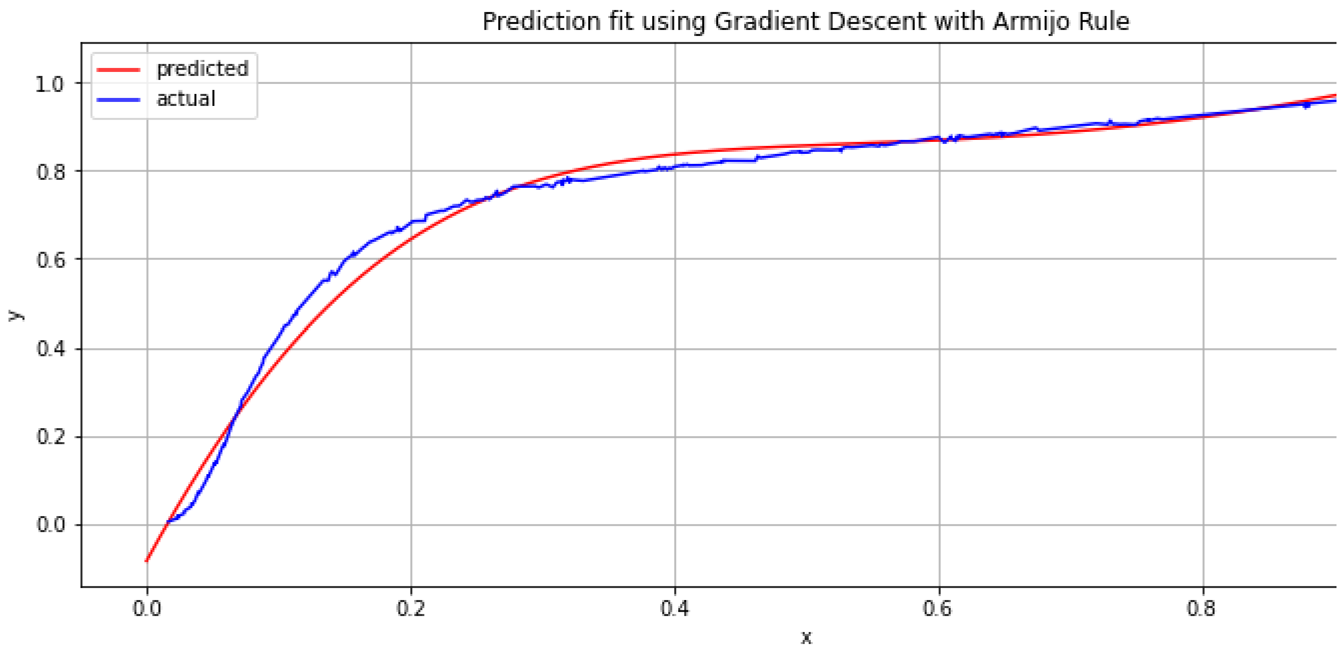
```
<matplotlib.legend.Legend at 0x7f3ec85f2f60>
```



Using he final estimate for `w` from the adaptive step-size plot the predicted values of the `yhat` vs. `x` usfor 1000 values `x` in `[0,1]`. On the same plot, plot `yhat` vs. `x` for the initial parameter `w=winit`. Also, plot `yts` vs. `xts`. You should see that gradient descent was able to improve the estimat slightly, although the initial estimate was not too bad.

```
# TODO
w2 = np.array(hist['w'])[10000-1,:]
xp = np.linspace(0,1,num=1000)
yhat = predict(w2,xp)
plt.figure(figsize=(13,5))
plt.plot(xp,yhat,'r')
plt.plot(x,y,'b')
plt.xlabel('x')
```

```
plt.ylabel('y')
plt.legend(('predicted','actual'))
plt.title('Prediction fit using Gradient Descent with Armijo Rule')
plt.grid()
```



Momentum Gradient Descent

This section is bonus.

One way to improve gradient descent is to use *momentum*. In momentum gradient descent, the update rule is:

```
f, fgrad = feval(w,...)
z = beta*z + fgrad
w = w - step*z
```

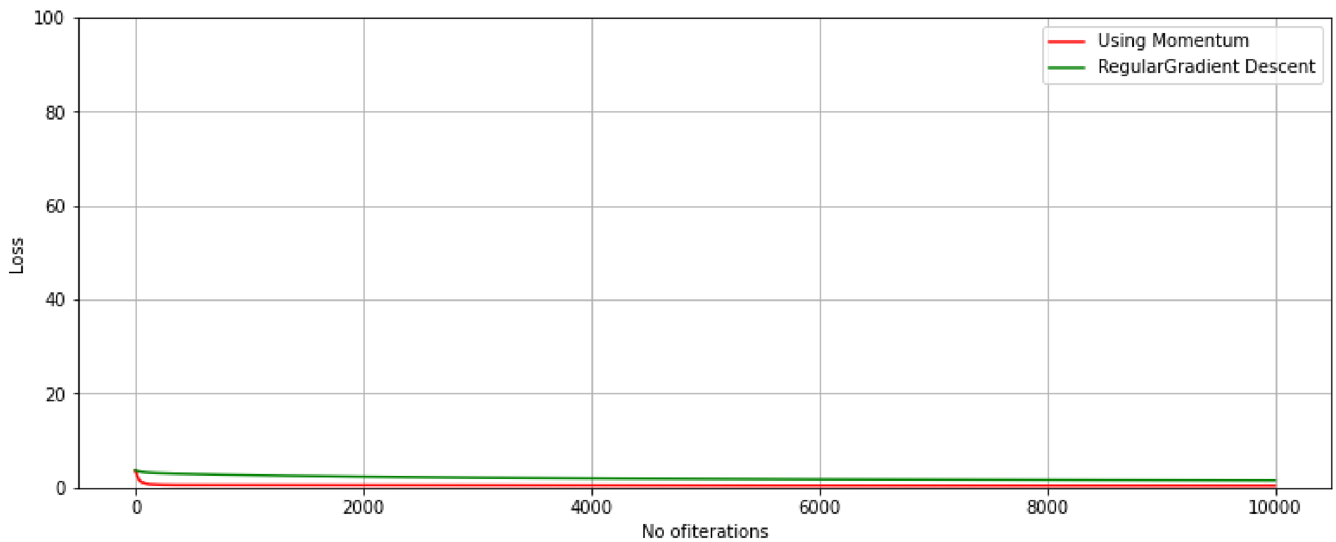
This is similar to gradient descent, except that there is a second order term on the gradient. Implement this algorithm with `beta = 0.99` and `step=1e-3`. Compare the convergence of the loss function with gradient descent.

```
# TODO
nit = 10000
step = 1e-5
beta = 0.99
z = np.zeros(np.shape(winit))
hist = {'w':[],'f':[]}
w3 = winit
for i in range(nit):
    f0, fgrad0 = feval(w3,xtr,ytr)
```

```
        f0, fgrad0 = feval(w3,xtr,ytr)
        z = z*beta + fgrad0
        w3 = w3 - z*step
        hist['w'].append(w3)
        hist['f'].append(f0)
    loss_momentum = np.array(hist['f'])


    # TODO
    # plot yhat vs. x
    plt.figure(figsize=(13,5))
    plt.plot(loss_momentum,'r-')
    plt.plot(loss,'g-')
    plt.xlabel('No ofiterations')
    plt.ylabel('Loss')
    plt.grid()
    plt.legend(('Using Momentum','RegularGradient Descent'))
    plt.ylim([0,100])
```

```
(0.0, 100.0)
```



Collaborated for this lab with Rebanta,Puneeet,anindya.

+ Code + Text

Beyond This Lab

In this lab, we have just touched at some of the ideas in optimization. There are several other important algorithms that you can explore:

- [Levenberg-Marquardt] method for non-linear least squares
- Newton's method
- More difficult non-linear least squares problems.