lab_nlls_soln

February 24, 2019

1 Lab: Nonlinear Least Squares for Modeling Materials

In this lab, we will explore gradient descent on nonlinear least squares. Suppose we wish to fit a model of the form,

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

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

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

where the summation is over training samples `(x_i,y_i)`. In general, this optimization has no closed-form expression. So gradient descent is widely used.

In this lab, we will implement gradient descent on nonlinear least squares in physical modeling of materials. Specifically, e we will estimate parameters for expansion of copper as a function of temperature. 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.

```
In [17]: import pandas as pd
         import numpy as np
         import matplotlib.pyplot as plt
         from sklearn.linear_model import Ridge, LinearRegression
```

1.1 Load the Data

The NIST agency has an excellent nonlinear regression website that has several datasets for trying nonlinear regression problem. 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 (unpublished}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.

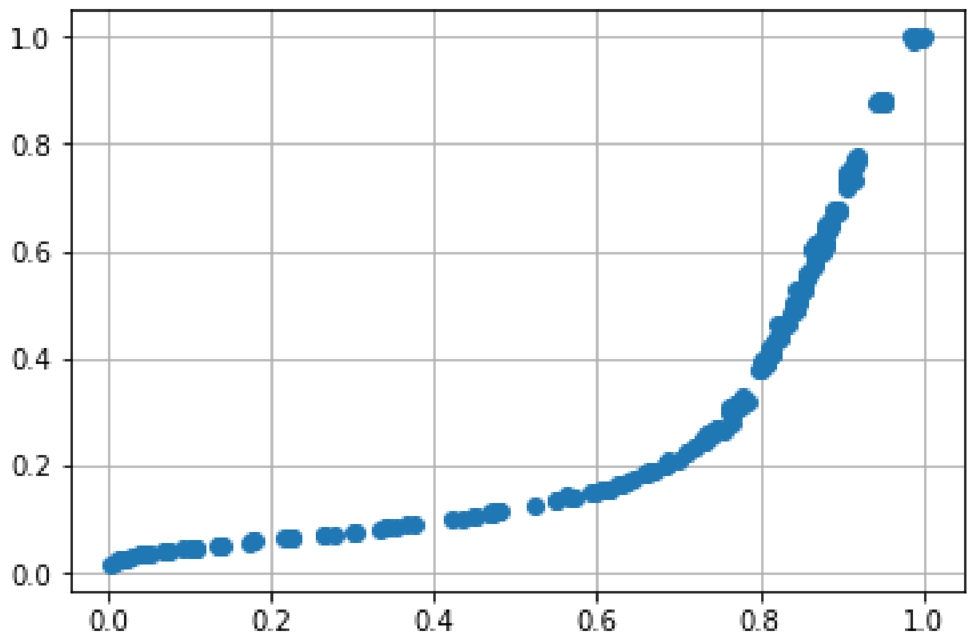
```
In [18]: url = 'https://itl.nist.gov/div898/strd/nls/data/LINKS/DATA/Hahn1.dat'
         df = pd.read_csv(url, skiprows=60, sep=' ',skipinitialspace=True, names=['x0','y0','du
         df.head()
```

Out[18]:

	x0	y0	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.

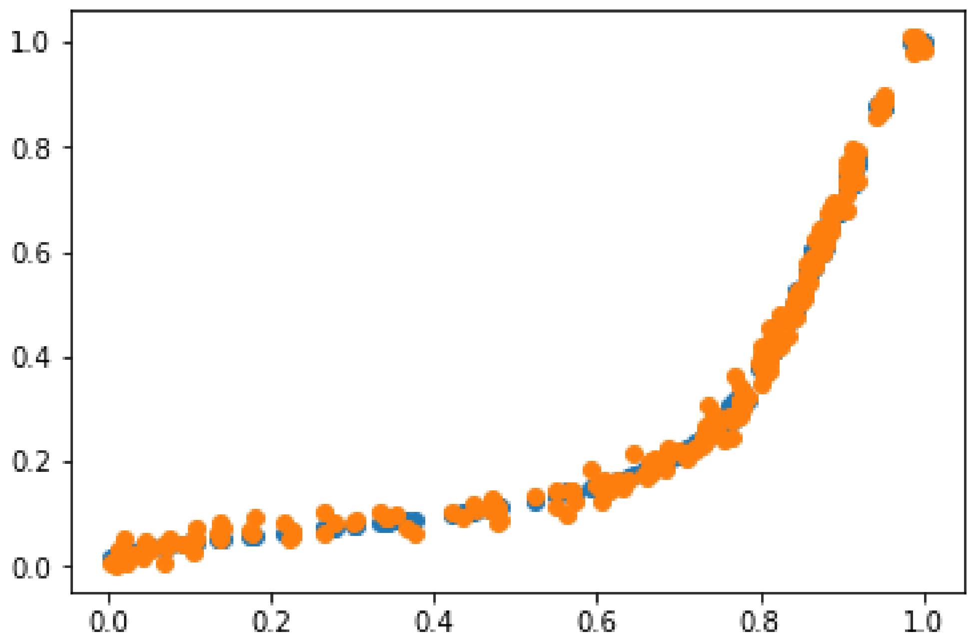
```
In [19]: # TODO
         # x0 = ...
         # y0 = ...
         # x0 = x0/np.max(x0)
         # y0 = y0/np.max(y0)
         # plt.plot(...)
         x0 = np.array(df['x0'])
         y0 = np.array(df['y0'])
         x = x0/np.max(x0)
         y = y0/np.max(y0)
         plt.plot(x,y,'o')
         plt.grid()
```



To make the problem a little more challenging, we will add some noise. Add random Gaussian noise with mean 0 and std. dev = 0.05 to y. Store the noisy results in yn. You can use the `np.random.normal()` function to add Gaussian noise. Plot yn vs. x.

```
In [20]: # TODO
         # yn = y + ...
         n = len(y0)
         yn = y + np.random.normal(0,0.02,n)

         plt.plot(x,y,'o')
         plt.plot(x,yn,'o')
```

```
Out[20]: [<matplotlib.lines.Line2D at 0x28edbc31a58>]
```



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.

```
In [21]: from sklearn.model_selection import train_test_split

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

1.2 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.

```
In [22]: def predict(w,x):

             # Get the length
             d = (len(w)-1)//2

             # TODO.  Extract a and b from w
             # a = ...
             # b = ...
             a = w[:d+1]
             b = w[d+1:]

             # TODO.  Compute yhat.  You may use the np.polyval function
             # But, remember you must flip the order the a and b
             # yhat = ...
             arev = a[::-1]
             brev = b[::-1]
             znum = np.polyval(arev,x)
             zden = 1+x*np.polyval(brev,x)
             yhat = znum/zden
             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 ]
```

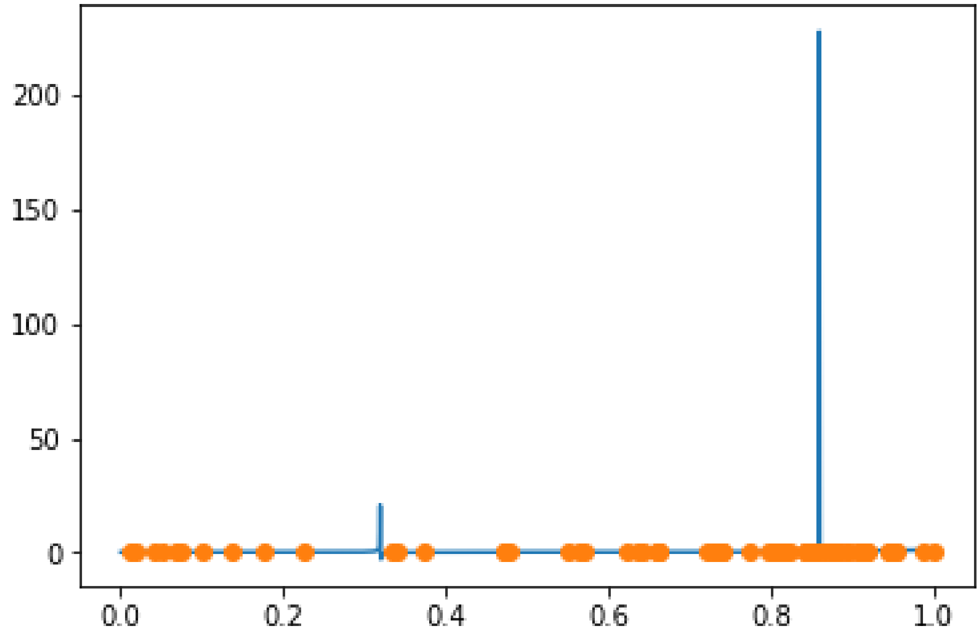
```
In [23]: d = 3

         # TODO.  Create the transformed feature matrix
         # Z = ...
         powd = np.arange(1,d+1)
```

```
Znum = xtr[:,None]**powd[None,:]
Zden = -ytr[:,None]*Znum
Z = np.hstack((Znum, Zden))

# TODO.  Fit with parameters with linear regression
# regr = LinearRegression()
# regr.fit(...)
regr = LinearRegression()
regr.fit(Z,ytr)

# TODO
# Extract the parameters from regr.coef_ and regr.intercept_ and store the parameter
# winit = ...
w0 = regr.coef_
a0 = regr.intercept_
winit = np.hstack((a0,w0))
```

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.

In [24]:
```
# TODO
# xp = ...
# yhat = ...
# plot(...)
xp = np.linspace(0,1,1000)
yhat  = predict(winit,xp)
plt.plot(xp,yhat)
plt.plot(xts, yts, 'o')
```

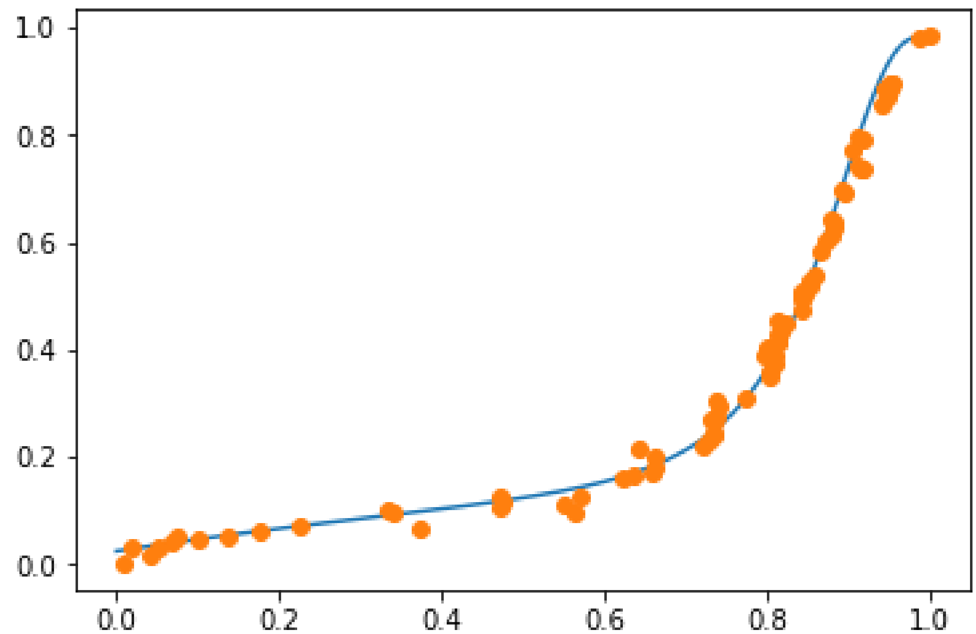
Out[24]: `[<matplotlib.lines.Line2D at 0x28edbca7828>]`



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.

In [25]:
```
# TODO.  Fit with parameters with linear regression
# regr = Ridge(alpha=1e-3)
# regr.fit(...)
regr = Ridge(alpha=1e-3)
regr.fit(Z,ytr)

# TODO
# Extract the parameters from regr.coef_ and regr.intercept_
# winit = ...
w0 = regr.coef_
a0 = regr.intercept_
winit = np.hstack((a0,w0))

# TODO
# Plot the results as above.
xp = np.linspace(0,1,1000)
yhat  = predict(winit,xp)
plt.plot(xp,yhat)
plt.plot(xts, yts, 'o')
```

Out[25]: [<matplotlib.lines.Line2D at 0x28edbd074a8>]



1.3 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)`.

```
In [26]: def feval(w,x,y):


             # TODO.  Parse w
             # a = ...
             # b = ...
             d = (len(w)-1)//2
             a = w[:d+1]
             b = w[d+1:]

             # TODO.  Znum[i,j] = x[i]**j
             pow1 = np.arange(0,d+1)
             Znum = x[:,None]**pow1[None,:]

             # TODO.  Zden[i,j] = x[i]**(j+1)
             pow2 = np.arange(1,d+1)
             Zden = x[:,None]**pow2[None,:]

             # TODO.  Compute yhat
             # Compute the numerator and denominator
             rnum = Znum.dot(a)
             rden = Zden.dot(b)
             yhat = rnum/(1+rden)

             # TODO.  Compute loss
             # f = ...
             e = yhat-y
             f = 0.5*np.sum(e**2)

             # TODO.  Compute gradients
             # fgrad = ...
             eden = e/(1+rden)
             dJ_da = eden.dot(Znum)
             enum = -e*yhat/(1+rden)
             dJ_db = enum.dot(Zden)
             fgrad = np.hstack((dJ_da, dJ_db))


             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.

```
In [27]: # TODO
         w0 = winit
         p = len(winit)
         w1 = w0 + np.random.normal(0,1,p)*1e-6
         f0, fgrad0 = feval(w0,xtr,ytr)
         f1, fgrad1 = feval(w1,xtr,ytr)

         print([f1-f0, fgrad0.dot(w1-w0)])
```

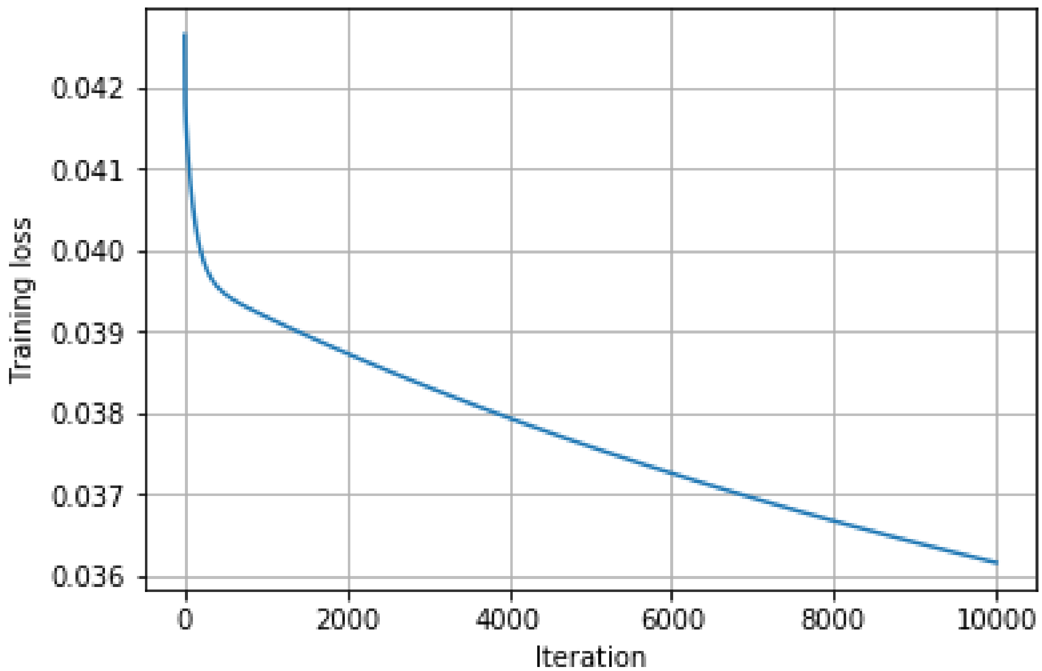
```
[7.116281790800483e-06, 7.1106249555072314e-06]
```

1.4 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.

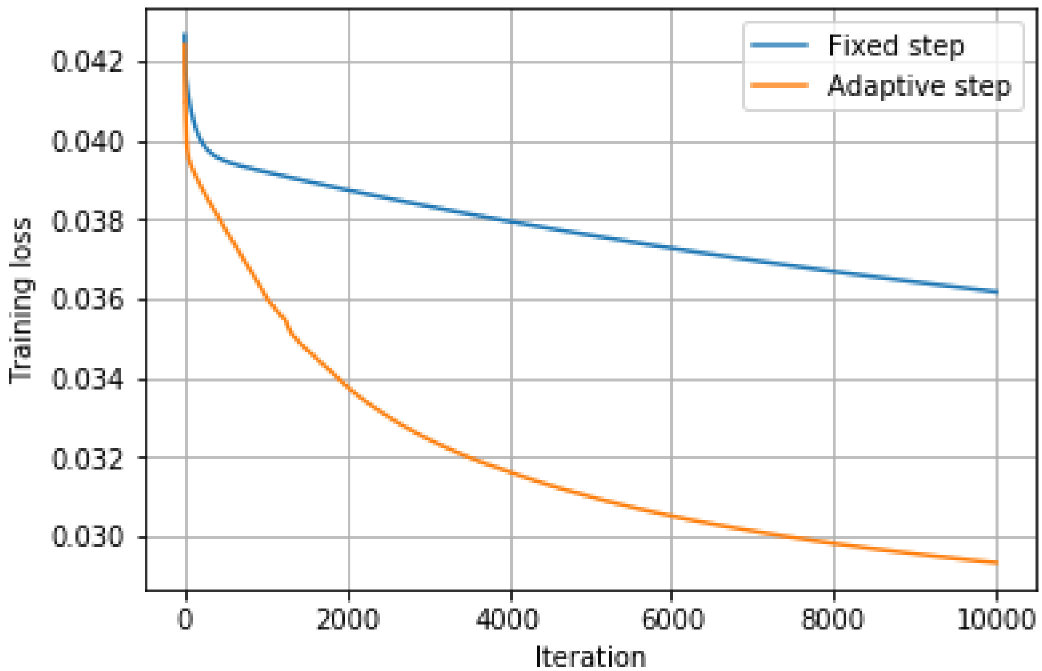
```
In [28]: nit = 10000
         step = 1e-6
         wt = winit
         fgd = np.zeros(nit)
         for it in range(nit):
             ft, fgradt = feval(wt,xtr,ytr)
             fgd[it] = ft
             wt  = wt - step*fgradt

         plt.plot(fgd)
         plt.xlabel('Iteration')
         plt.ylabel('Training loss')
         plt.grid()
```



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.

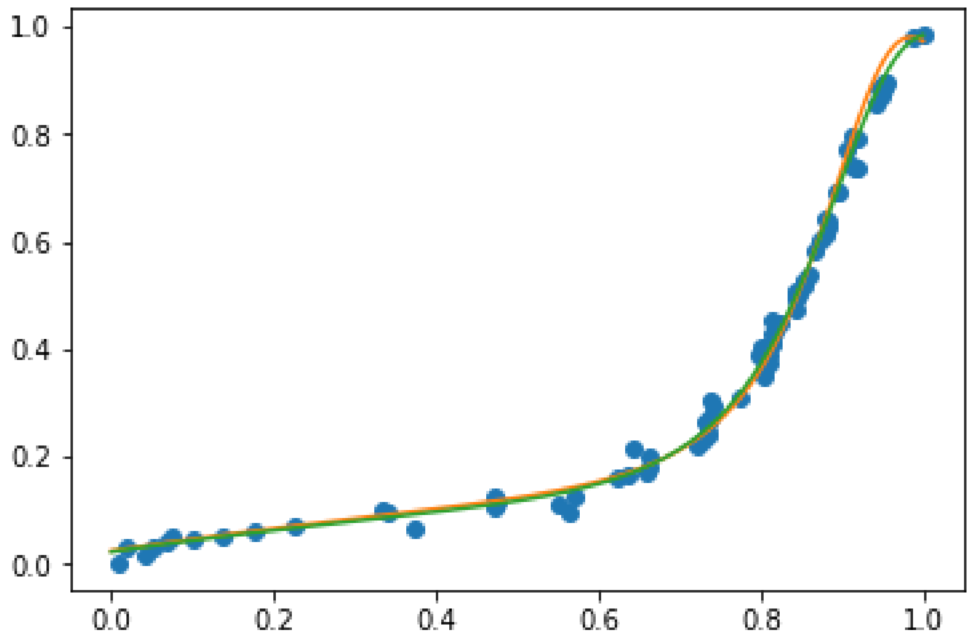
In [29]:
```
nit = 10000
step = 1e-6  # Initial step
w0 = winit
fadapt = np.zeros(nit)
f0, fgrad0 = feval(w0,xtr,ytr)
for it in range(nit):

    # Compute test point
    w1 = w0 - step*fgrad0
    f1, fgrad1 = feval(w1,xtr,ytr)

    # Test Armijo rule
    alpha = 0.5
    if (f1-f0 < alpha*fgrad0.dot(w1-w0)) and (f1 < f0):
        step = step*2
        f0 = f1
        fgrad0 = fgrad1
        w0 = w1
    else:
        step = 0.5*step
```

```
        fadapt[it] = f0


    plt.plot(fgd)
    plt.plot(fadapt)
    plt.xlabel('Iteration')
    plt.ylabel('Training loss')
    plt.legend(['Fixed step', 'Adaptive step'])
    plt.grid()
```



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.

```
In [30]: xp = np.linspace(0,1,500)
         yinit = predict(winit,xp)
         yhat = predict(w0,xp)
         plt.plot(xts,yts,'o')
         plt.plot(xp,yinit,'-')
         plt.plot(xp,yhat,'-')

Out[30]: [<matplotlib.lines.Line2D at 0x28edce39978>]
```



1.5 Momentum Gradient Descent

This section is bonus.

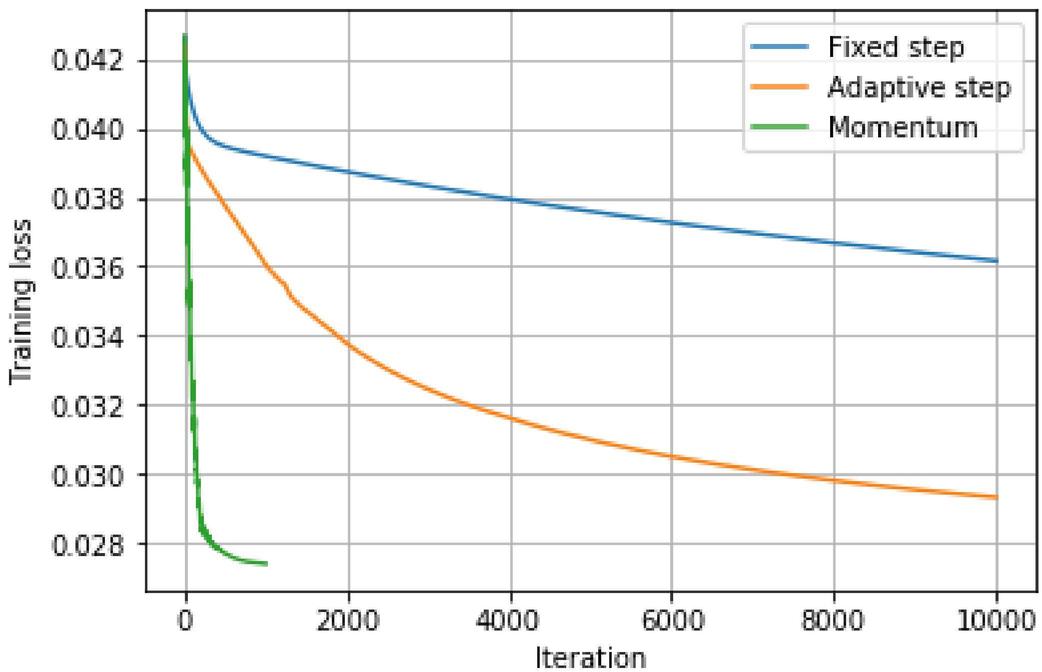
One way to improve gradient descent is to use *momentum*. In momentum gradient descent, the update rule is:

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

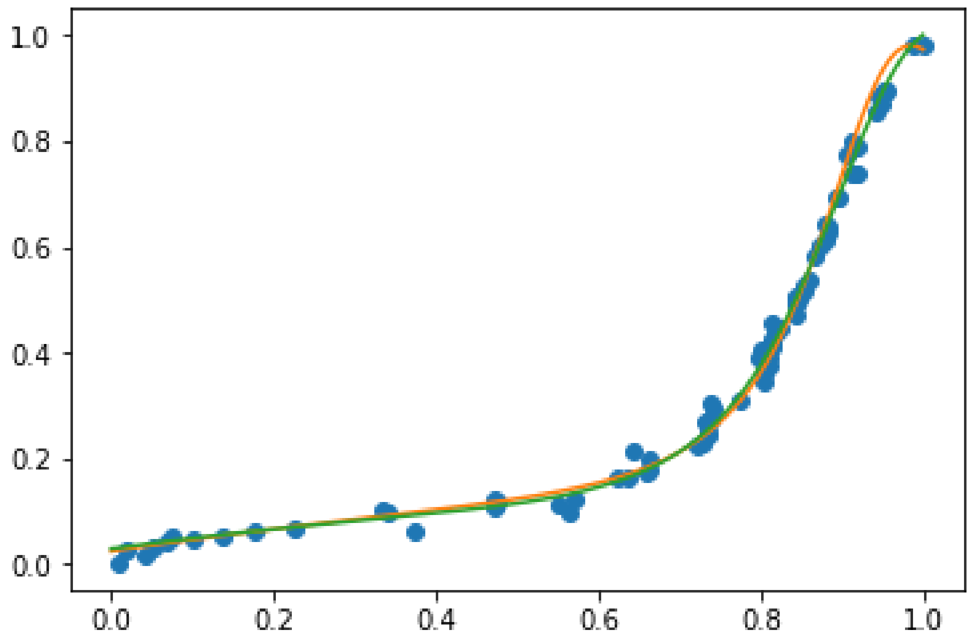
This is similar to gradient descent, except that there is a second order term on the gradient. Implement this algorithm with `beta = 0.99` and `step=1e-5`. Compare the convergence of the loss function with gradient descent.

```
In [31]: nit = 1000
         step = 1e-5
         beta = 0.99
         wt = winit
         p = len(winit)
         z = np.zeros(p)
         fmom = np.zeros(nit)
         for it in range(nit):
             ft, fgradt = feval(wt,xtr,ytr)
             z = beta*z + fgradt
             wt  = wt - step*z
             fmom[it] = ft
```

```
plt.plot(fgd)
plt.plot(fadapt)
plt.plot(fmom)
plt.xlabel('Iteration')
plt.ylabel('Training loss')
plt.legend(['Fixed step', 'Adaptive step', 'Momentum'])
plt.grid()
```




```
In [32]: xp = np.linspace(0,1,500)
         yinit = predict(winit,xp)
         yhat = predict(wt,xp)
         plt.plot(xts,yts,'o')
         plt.plot(xp,yinit,'-')
         plt.plot(xp,yhat,'-')

Out[32]: [<matplotlib.lines.Line2D at 0x28edcf15c88>]
```




```
In [ ]:
```

```
In [ ]:
```