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March 21, 2022

1 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.

[1]:
```
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 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 (unpublished}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.

[2]:
```
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()
```

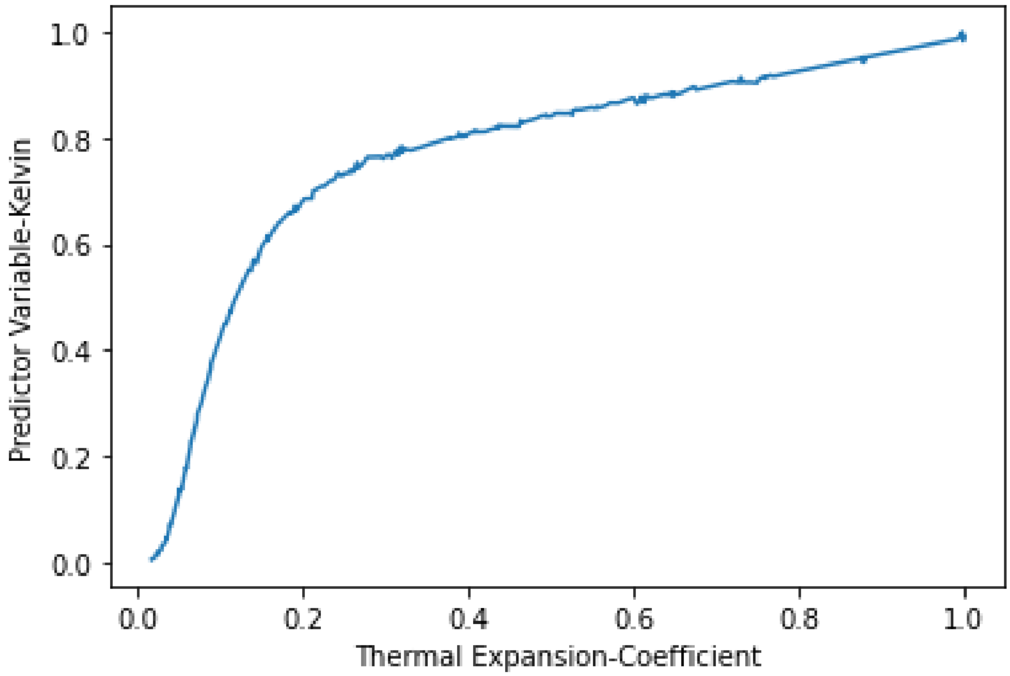
[2]:

	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`.

[3]:
```
x0 = np.array(df['x0'])
y0 = np.array(df['y0'])
x = x0/np.max(x0)
y = y0/np.max(y0)
args = np.argsort(x)
x = x[args]
y = y[args]
plt.plot(x,y)
plt.xlabel('Thermal Expansion-Coefficient')
plt.ylabel('Predictor Variable-Kelvin')
```

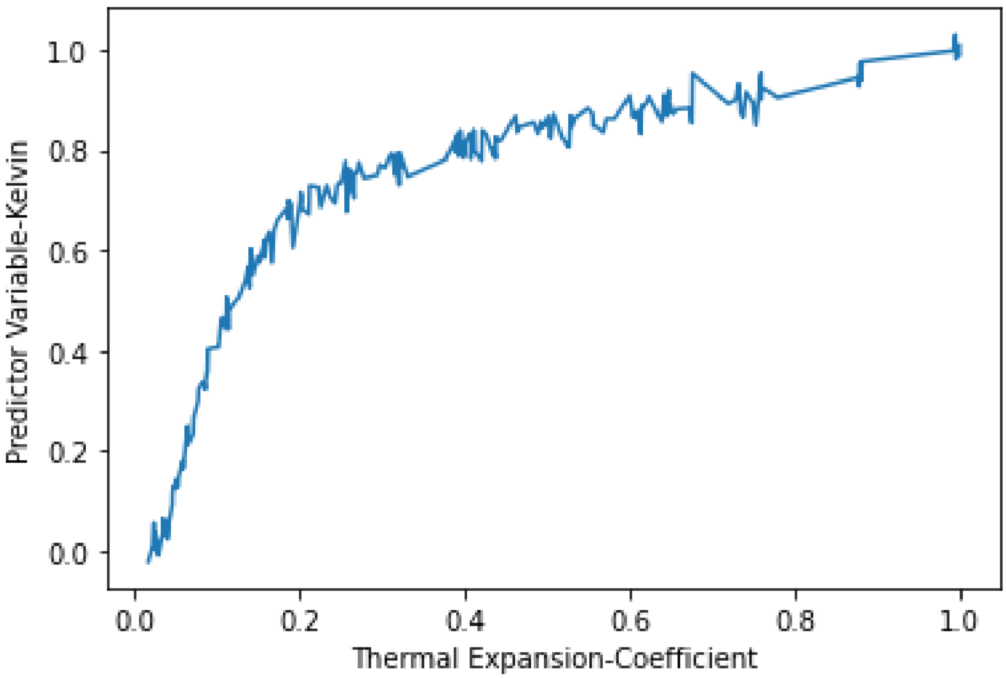
[3]:
```
Text(0, 0.5, 'Predictor Variable-Kelvin')
```



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`.

[4]:
```
yn = y+np.random.normal(0,0.02,y.shape)
plt.plot(x,yn)
plt.xlabel('Thermal Expansion-Coefficient')
plt.ylabel('Predictor Variable-Kelvin')
```

[4]:
```
Text(0, 0.5, 'Predictor Variable-Kelvin')
```



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.

[5]:
```
from sklearn.model_selection import train_test_split

# TODO 3
xtr, xts, ytr, yts = train_test_split(x,yn,test_size=0.33,shuffle=True)
args = np.argsort(xtr)
args_t = np.argsort(xts)
xtr = xtr[args]
ytr = ytr[args]
xts = xts[args_t]
yts = yts[args_t]
```

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.

[6]:
```python
def predict(w,x):
  d = (len(w)-1)//2
  a = w[:d+1]
  b = w[d+1:]
  a = np.flip(a)
  b = np.append(np.flip(b),1)
  yhat = np.polyval(a,x)/(np.polyval(b,x))
  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 ]
```

[7]:
```python
d = 3

# TODO 6.  Create the transformed feature matrix
# Z = ...

# TODO 7.  Fit with parameters with linear regression
# regr = LinearRegression()
# regr.fit(...)

# TODO 8
# Extract the parameters from regr.coef_ and regr.intercept_ and store the␣
 ↪parameter vector in winit
# winit = ...
dp = np.arange(1,d+1)
Z = np.zeros((len(xtr),2*d))
for i in range(len(xtr)):
  Z[i,:] = np.concatenate((np.power(xtr[i],dp),ytr[i]*np.power(xtr[i],dp)))
regr = LinearRegression()
regr.fit(Z,ytr)
a = np.append([regr.intercept_],regr.coef_[0:d])
b = -regr.coef_[d:]
winit = np.append(a,b)
print(winit)
```

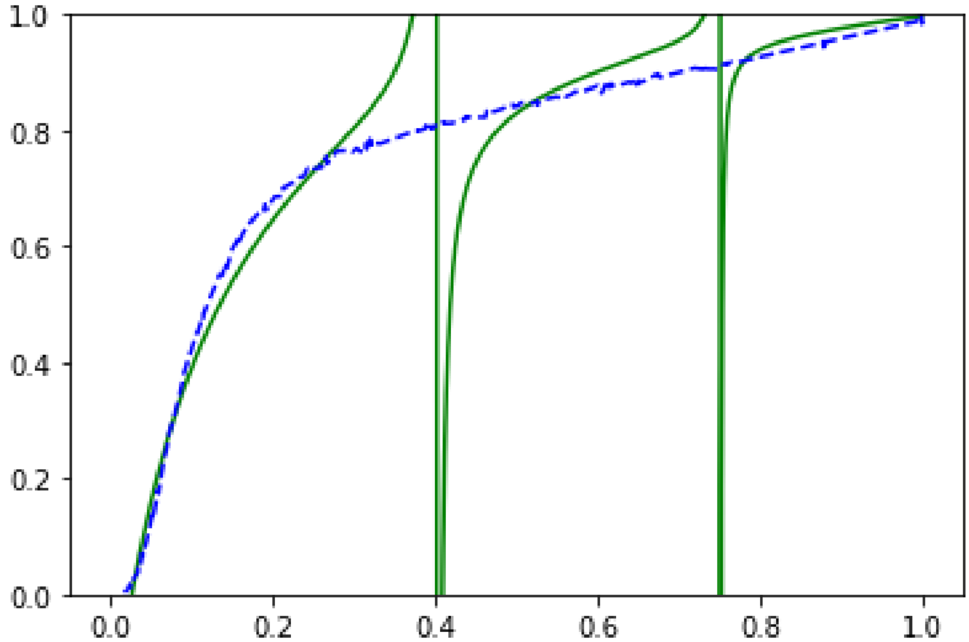
```
[ -0.2488037   10.39530813 -36.51161145  30.74692537   4.10824682
 -26.95841352  26.24604627]
```

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.

[8]:

```python
# TODO 9
# xp = ...
# yhat = ...
# plot(...)
xp = np.linspace(0,1,1000)
yhat = predict(winit,xp)
plt.plot(xp,yhat,'g',x,y,'b--')
plt.ylim([0,1])
```

[8]: (0.0, 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.

[9]:

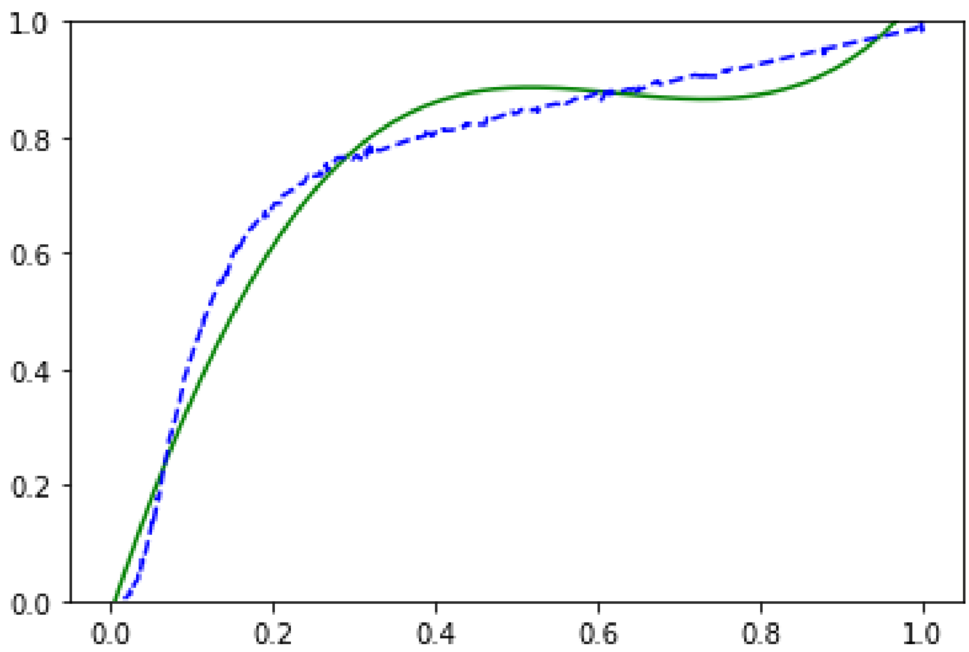
```python
# TODO 10.  Fit with parameters with linear regression
# regr = Ridge(alpha=1e-3)
# regr.fit(...)

# TODO 11
# Extract the parameters from regr.coef_ and regr.intercept_
# winit = ...

# TODO 12
# Plot the results as above.
rigregr = Ridge(alpha=1e-3)
```

```
rigregr.fit(Z,ytr)
a = np.concatenate(([rigregr.intercept_],rigregr.coef_[0:d]))
b = -rigregr.coef_[d:]
winit = np.append(a,b)
xp = np.linspace(0,1,1000)
yhat = predict(winit,xp)
plt.plot(xp,yhat, 'g',x,y, 'b--')
plt.ylim(0,1.0)
```

[9]: (0.0, 1.0)



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)`.

[10]:
```
def feval(w,x,y):
  d = (len(w)-1)//2
  a = w[0:d+1]
  b = w[d+1:]
  Znum = np.zeros((len(x),d+1))
  for j in range(d+1):
    Znum[:,j] = x[:]**j
```

```
  Zden = np.zeros((len(x),d))
  for j in range(d):
    Zden[:,j] = x[:]**(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.

[11]:
```
# TODO 19
w0 = winit
f0, fgrad0 = feval(w0,xtr,ytr)
r1 = 1e-6
wl = w0 + r1
fl,fgradl = feval(wl,xtr,ytr)
print("Actual fl-f0 = %12.4e" % (fl-f0))
print("Predicted fl-f0 = %12.4e" % (fgrad0.dot(wl-w0)))
```

```
Actual fl-f0 =  -2.8351e-07
Predicted fl-f0 =  -2.8362e-07
```

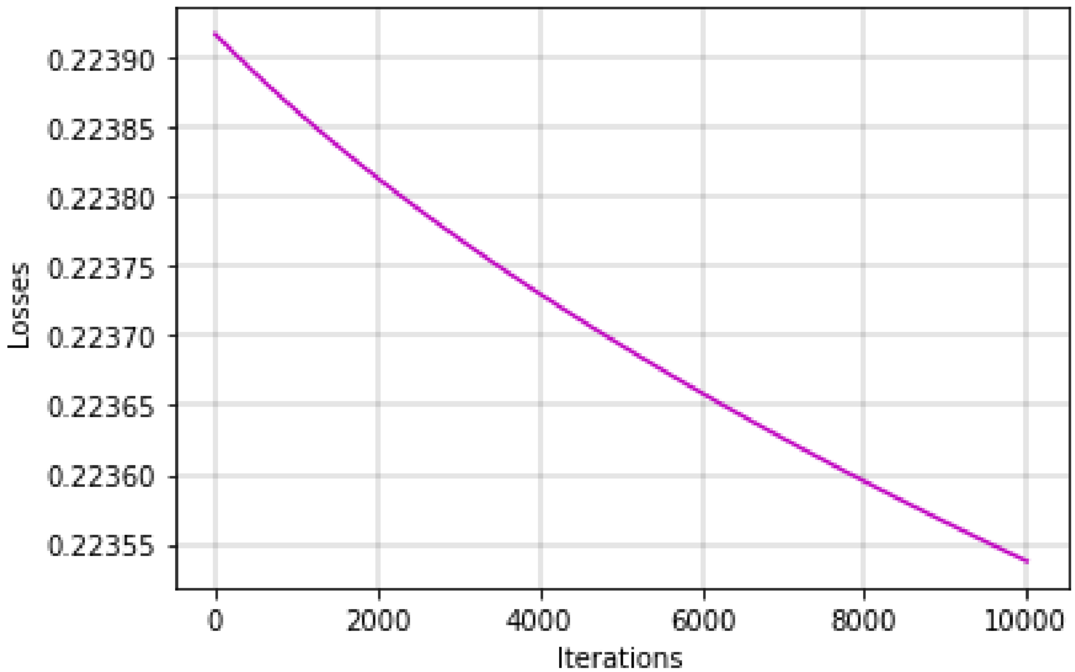
1.4 Implement gradient descent

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.

[12]:
```
# TODO 20
# fgd = ...
nit = 10000
step = 1e-6
nit = 10000
step = 1e-6
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)
loss = np.array(hist['f'])
plt.plot(loss, 'm-')
plt.xlabel('Iterations')
plt.ylabel('Losses')
plt.grid(color='k',linewidth=0.2)
```

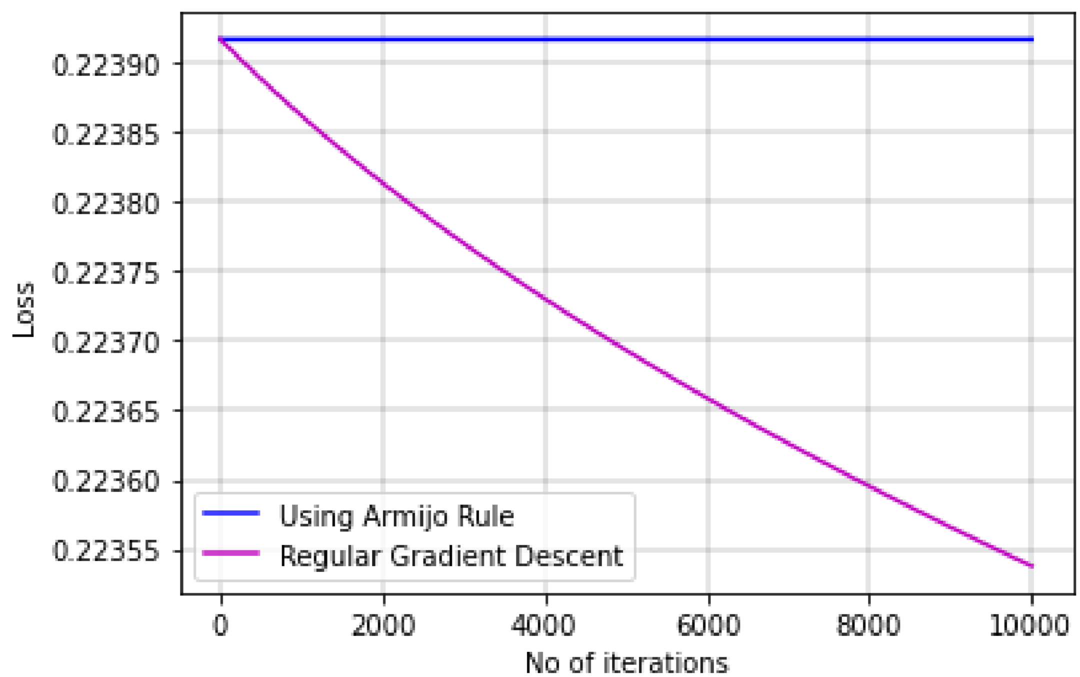


Now, try to get a faster convergence with adaptive step-size using the Armijo rule. Implement the gradient descent with adaptive step size. Let `fadapt[it]` be the loss function on iteration `it`. Plot `fadapt[it]` and `fgd[it]` vs. `it` on the same graph. You should see a slight improvement, but not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

[16]:
```
# TODO 21
# fadapt = ...
nit= 10000
step= 1e-6
hist= {'w':[],'f':[]}
w0 = winit
f0, fgrad0 = feval(winit,xtr,ytr)
for i in range(nit):
    w1 = w0 - fgrad0*step
    f1, fgradl = feval(wl,xtr,ytr)
```

```
    df = fgrad0.dot(w1-w0)
    al= 0.5
    if (f1-f0 < al*df) and (fl<f0):
        step= step*2
        f0 = fl
        fgrad0 = fgradl
        w0 = wl
    else:
        step= step/2
        hist['w'].append(w0)
        hist['f'].append(f0)
loss_arm = np.array(hist['f'])
plt.plot(loss_arm,'b-')
plt.plot(loss,'m-')
plt.xlabel('No of iterations')
plt.ylabel('Loss')
plt.grid(color='k',linewidth=0.2)
plt.gca().legend(('Using Armijo Rule','Regular Gradient Descent'))
```

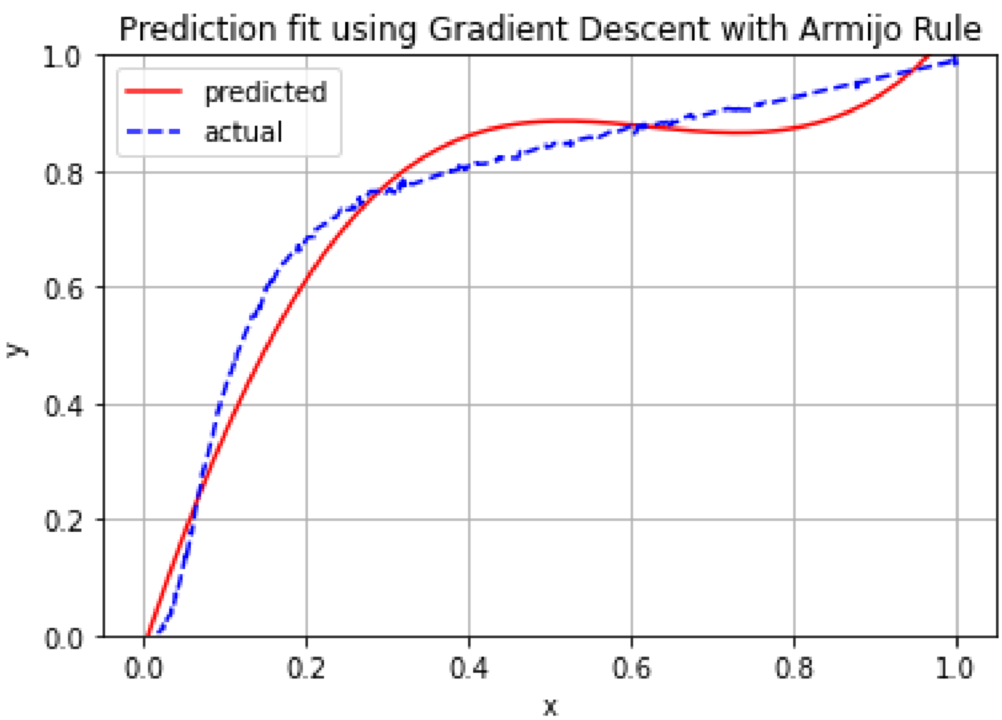
[16]: <matplotlib.legend.Legend at 0x23875327970>



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.

[19]:
```python
# TODO 22
# xp = np.linspace(...)
# yhat = ...
# plot(...)
w_adapt_fin = np.array(hist['w'])[9998,:]
xp = np.linspace(0,1,num=1000)
yhat = predict(w_adapt_fin,xp)
plt.plot(xp,yhat, 'r')
plt.plot(x,y, 'b--')
plt.xlabel( 'x')
plt.ylabel( 'y')
plt.gca().legend(('predicted','actual'))
plt.title('Prediction fit using Gradient Descent with Armijo Rule')
plt.grid()
plt.ylim(0,1)
```

[19]: (0.0, 1.0)



1.5 Momentum Gradient Descent

This section is bonus.

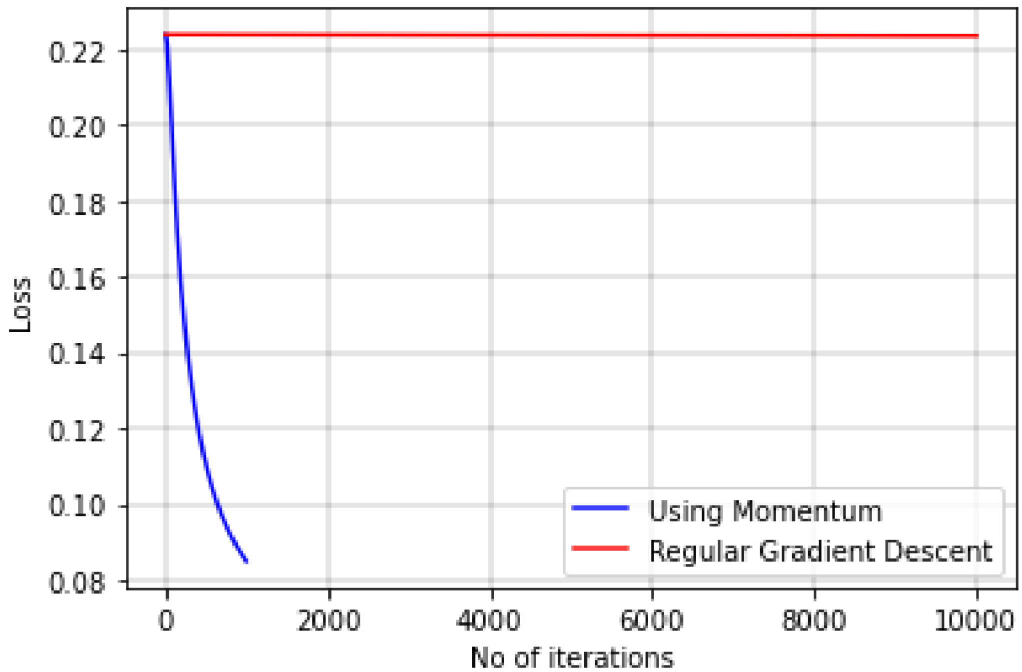
One way to improve gradient descent is to use *momentum*. In momentum gradient descent, the update rule is:

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

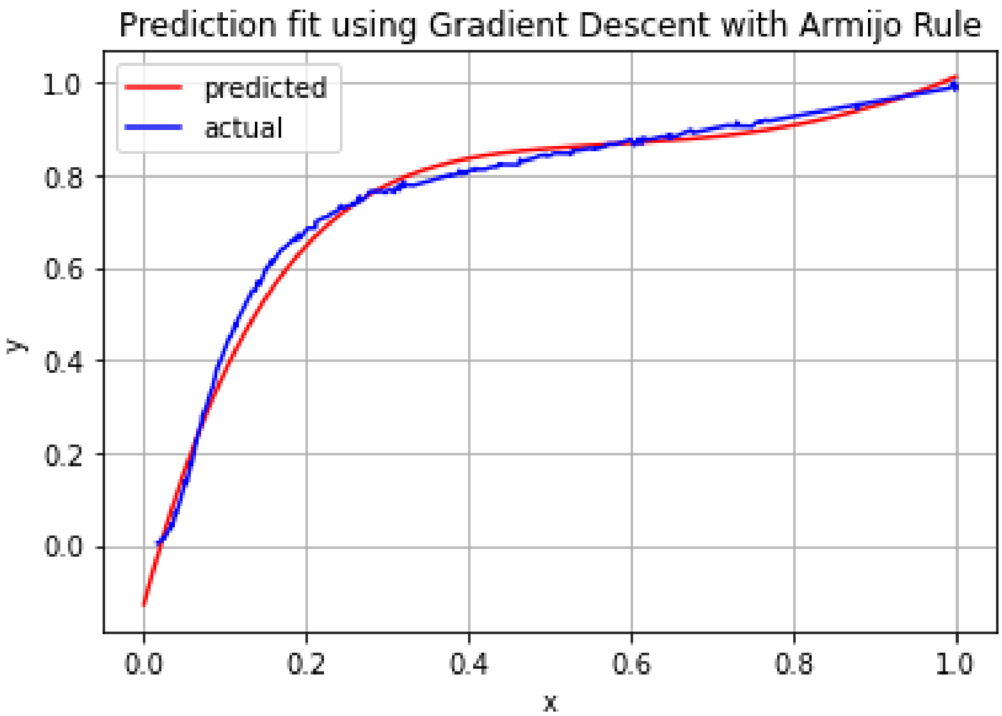
This is similar to gradient descent, except that there is a second order term on the gradient. Implement this algorithm with `beta = 0.99` and `step=1e-3`. Compare the convergence of the loss function with gradient descent.

[20]:
```
# TODO 23
nit = 1000
step = 1e-3
beta = 0.99
z = np.zeros(np.shape(winit))
hist = {'w':[],'f':[]}
w0 = winit
for i in range(nit):
    f0, fgrad0 = feval(w0,xtr,ytr)
    z = z*beta + fgrad0
    w0 = w0 - z*step
    hist['w'].append(w0)
    hist['f'].append(f0)
loss_mom = np.array(hist['f'])
plt.plot(loss_mom, 'b-')
plt.plot(loss,'r-')
plt.xlabel('No of iterations')
plt.ylabel('Loss')
plt.grid(color='k',linewidth=0.2)
plt.gca().legend(('Using Momentum','Regular Gradient Descent'))
```

[20]:
```
<matplotlib.legend.Legend at 0x23875193580>
```



[21]:
```
# TODO 24
# plot yhat vs. x
w_mom = np.array(hist['w'])[999,:]
xp = np.linspace(0,1,num=1000)
yhat = predict(w_mom,xp)
plt.plot(xp,yhat, 'r')
plt.plot(x,y, 'b')
plt.xlabel( 'x')
plt.ylabel( 'y')
plt.gca().legend(('predicted','actual'))
plt.title('Prediction fit using Gradient Descent with Armijo Rule')
plt.grid()
```



1.6 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.

[ ]:

```

```