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.

In [1]:

```
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 (https://www.itl.nist.gov/div898/strd/nls/nls_main.shtml) 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 (unpublished}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.

In [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=['x0','y0','dummy'])
df.head()
```

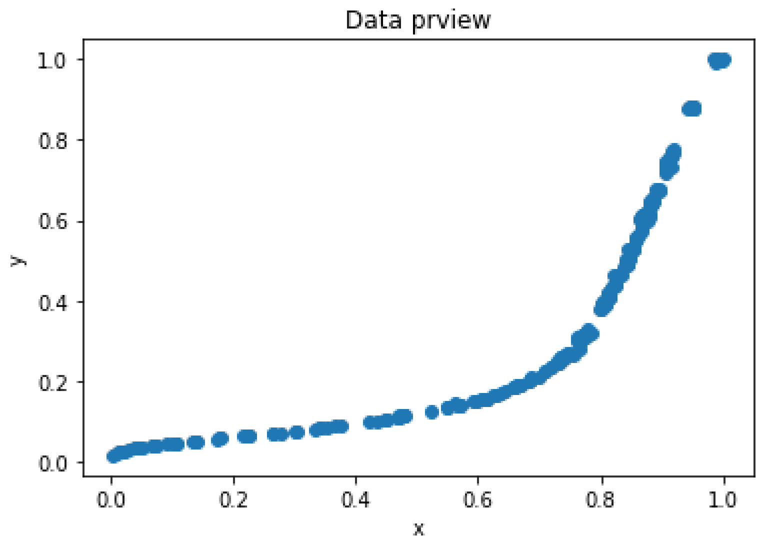
Out[2]:

	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 [3]:

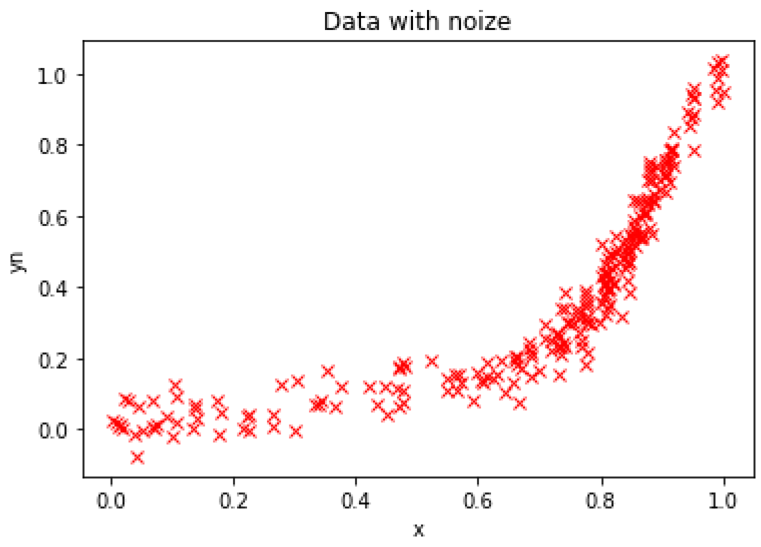
```
# TODO
# x0 = ...
# y0 = ...
# x = x0/np.max(x0)
# y = y0/np.max(y0)
# plt.plot(...)
x0 = df['x0'].values
y0 = df['y0'].values
x = x0/np.max(x0)
y = y0/np.max(y0)
plt.plot(x, y, 'o')
plt.title('Data prview')
plt.xlabel('x')
plt.ylabel('y')
plt.show()
```



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 [4]:

```
# TODO
# yn = y + ...
yn = y + np.random.normal(0, 0.05, y.shape)
plt.plot(x, yn, 'xr')
plt.title('Data with noize')
plt.xlabel('x')
plt.ylabel('yn')
plt.show()
```



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 [5]:

```
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)
```

Initial Fit for a Rational Model

The NIST website (https://www.itl.nist.gov/div898/strd/nls/data/hahn1.shtml) 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 [6]:

```
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:]
    b_ = np.append([1], b)
    # TODO.  Compute yhat.  You may use the np.polyval function
    # But, remember you must flip the order the a and b
    # yhat = ...
    yhat = np.polynomial.polynomial.polyval(x, a)/np.polynomial.polynomial.polyval(x, 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 ]
```

In [7]:

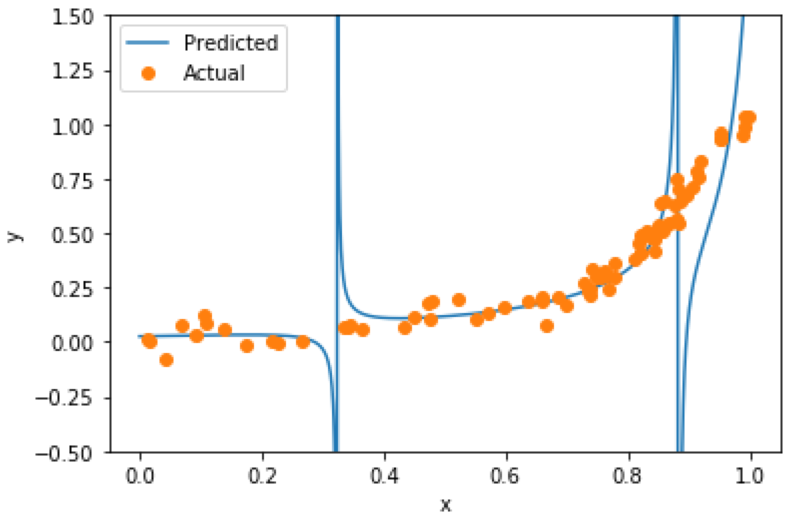
```
d = 3

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

exp_index = np.arange(d) + 1

X_d = np.power(xtr[:, None], exp_index)

Z = np.hstack((X_d, -X_d * ytr[:, None]))

# Note: Here inside of using Z giving in the instruction, I use Z that add minus to last half, so
# Z[i,:] = [ x[i], ... , x[i]**d, -y[i]*x[i], ... , -y[i}*x[i]**d ] to give the correct sign symbc


# 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 vector in wir
# winit = ...
winit = np.append(regr.intercept_, regr.coef_)
print(winit)
# X_d
# Z[1]
```

```
[ 0.0256423  -0.0826421  -0.06394733  0.13870306 -5.19179191  7.5905407
 -3.38995231]
```

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 [8]:

```
# TODO
# xp = ...
# yhat = ...
# plot(...)

xp = np.arange(0, 1, 0.001)
yhat = predict(winit, xp)
plt.plot(xp, yhat)
plt.plot(xts, yts, 'o')
plt.legend(['Predicted', 'Actual'])
plt.xlabel('x')
plt.ylabel('y')
plt.ylim([-0.5, 1.5])
plt.show()
```



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 [9]:

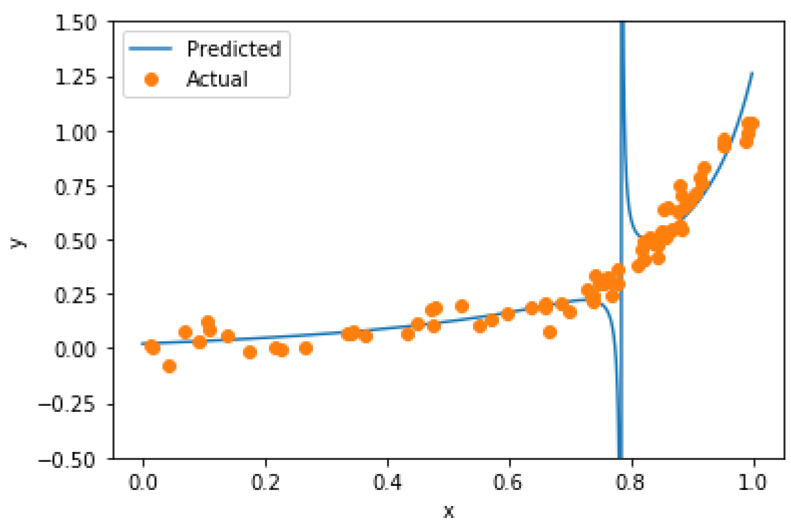
```
# TODO.  Fit with parameters with linear regression
# regr = Ridge(alpha=1e-3)
# regr.fit(...)

regr = Ridge(alpha=1e-3)
regr.fit(Z, ytr)

# TODO
# Extract the parameters from regr.coef_ and regr.intercept_
# winit = ...
winit = np.append(regr.intercept_, regr.coef_)
winit
# TODO
# Plot the results as above.
```

Out[9]:

```
array([ 0.02066477,  0.06794623, -0.09330935, -0.03734697, -1.98780269,
        0.74236424,  0.21239623])
```

In [10]:

```
yhat = predict(winit, xp)
plt.plot(xp, yhat)
plt.plot(xts, yts, 'o')
plt.legend(['Predicted', 'Actual'])
plt.xlabel('x')
plt.ylabel('y')
plt.ylim([-0.5, 1.5])
plt.show()
```



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 [11]:

```
def feval(w,x,y):


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

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

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

    # TODO.  Compute yhat
    # Compute the numerator and denominator
    yhat = np.sum(Znum * a, axis=1)/np.sum(Zden * b_, axis=1)

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

    # TODO.  Compute gradients
    # fgrad = ...

    f_a = np.sum(Znum * ((yhat - y)/ np.sum(Zden * b_, axis=1))[:, None], axis=0)


    f_b = np.sum( Zden[:, 1:] * ((y - yhat) * yhat /np.sum(Zden * b_, axis=1))[:, None], axis=0)

    fgrad = np.hstack((f_a, f_b))

    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 [12]:

```
# TODO
w0 = np.copy(winit)
f0, fgrad0 = feval(w0, xtr, ytr)
w1 = np.copy(w0)
w1 *= 1.0001
# print(winit)
f1, fgrad1 = feval(w1, xtr, ytr)
print("f1 - f0: ", f1 - f0)
# print(fgrad0,'\n' ,fgrad1)
print("Predicted: ",np.dot(fgrad0, (w1 - w0)))
```

```
f1 - f0:  -26.822713357279714
Predicted:  -53.986523711620436
```

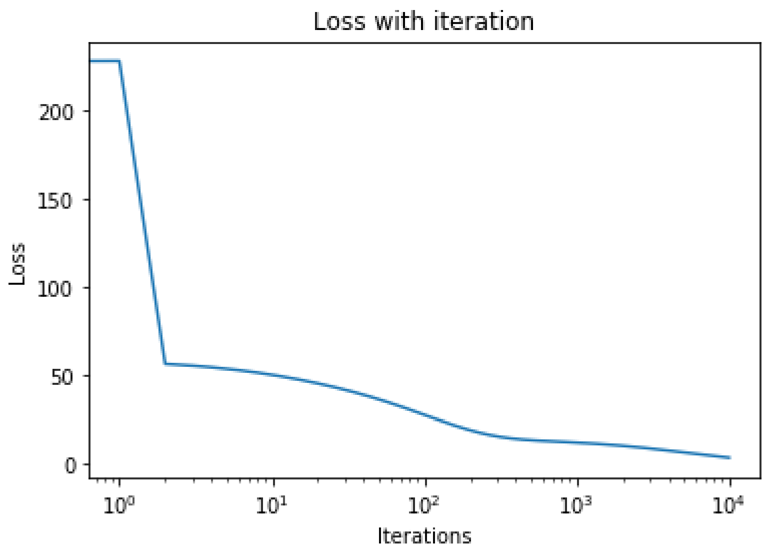
Implement gradient descent

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 [13]:

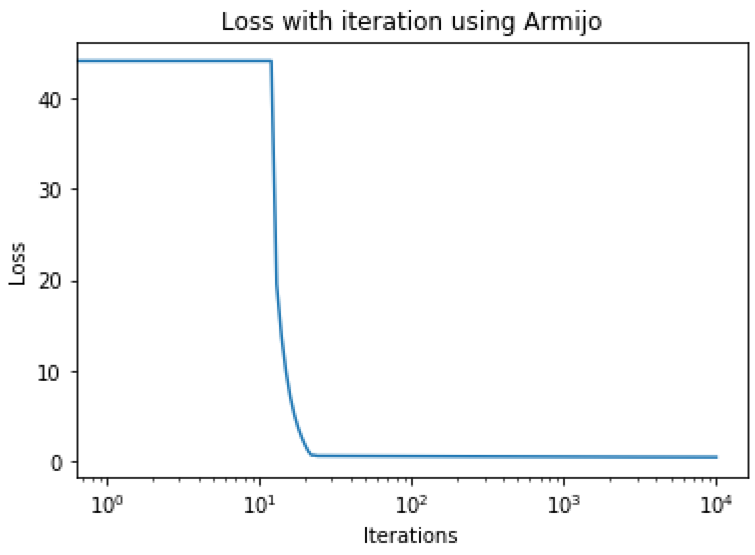
```
# TODO
# fgd = ...
nit = 10000
step = 1e-6
w0 = np.copy(winit)
fgd = []
for i in range(nit):
    f0, fgrad0 = feval(w0, xtr, ytr)
    w0 = w0 - step*fgrad0
    fgd.append(f0)
plt.semilogx(fgd)
plt.xlabel('Iterations')
plt.ylabel('Loss')
plt.title('Loss with iteration')
plt.show()
```



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 [14]:

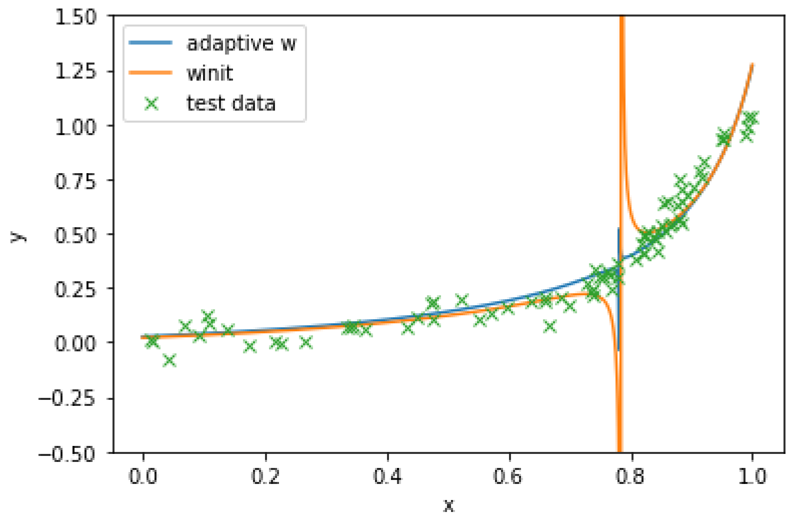
```
# TODO
# fadapt = ...
nit = 10000
step = 1e-6  # Initial step
fadapt = []
w0 = np.copy(winit)
f0, fgrad0 = feval(w0, xtr, ytr)

for i in range(nit):

    w1 = w0 - step*fgrad0
    f1, fgrad1 = feval(w1, xtr, ytr)

    df_est = fgrad0.dot(w1 - w0)
    alpha = 0.5
    if (f1-f0 < alpha * df_est) and (f1 < f0):
        step = step*2
        f0 = f1
        fgrad0 = fgrad1
        w0 = w1
    else:
        step = step/2

    fadapt.append(f0)

plt.semilogx(fadapt)
plt.xlabel('Iterations')
plt.ylabel('Loss')
plt.title('Loss with iteration using Armijo')
plt.show()
```



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 [15]:

```
# TODO
# xp = np.linspace(...)
# yhat = ...
# plot(...)
xp = np.linspace(0, 1, 1000)
yhat = predict(w0, xp)
yhat_init = predict(winit, xp)
plt.plot(xp, yhat)
plt.plot(xp, yhat_init )
plt.plot(xts, yts, 'x')
plt.legend(['adaptive w', 'winit', 'test data'])
plt.xlabel('x')
plt.ylabel('y')
plt.ylim(-0.5, 1.5)
plt.show()
```



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
```

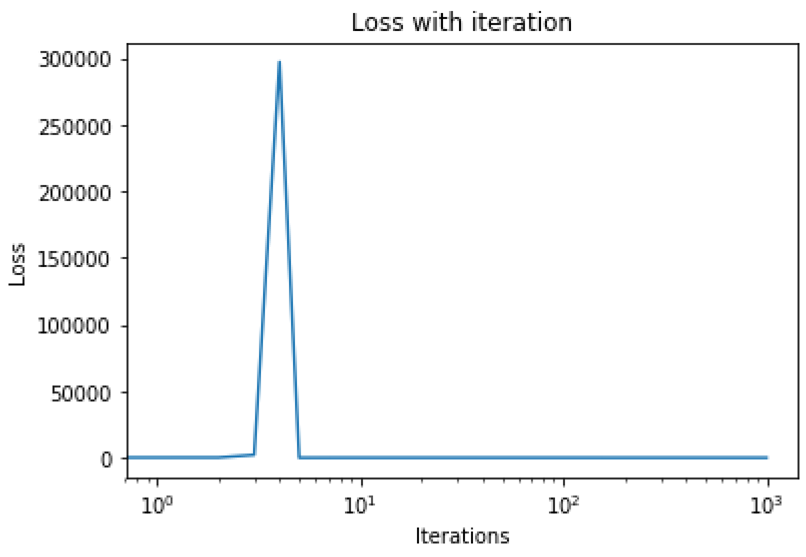
This is similar to gradient descent, except that there is a second order term on the gradient. Implement this algorithm with `beta = 0.99` and `step=1e-5` . Compare the convergence of the loss function with gradient descent.

In [16]:

```
# TODO
nit = 1000
step = 1e-5
beta = 0.99

w0 = np.copy(winit)
z = np.zeros(w0.shape)
fgd = []
for i in range(nit):
    f0, fgrad0 = feval(w0, xtr, ytr)
    z = beta*z + fgrad0
    w0 = w0 - step*z
    fgd.append(f0)
```

In [17]:

```
# TODO
# plot yhat vs. x
plt.semilogx(fgd)
plt.xlabel('Iterations')
plt.ylabel('Loss')
plt.title('Loss with iteration')
plt.show()
```



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 (https://en.wikipedia.org/wiki/Levenberg%E2%80%93Marquardt_algorithm) method for non-linear least squares
- Newton's method
- More difficult non-linear least squares problems.

In [ ]:

```
```