L7_Regression_filled

January 25, 2019

0.1 Part 1 simple linear regression

0.1.1 To do

- Explain w/partner each line in this notebook and execute each cell
- Explore relationship between quality of prediction and (size of training set / noise level)
  - Specifically discuss how you would automate this searching

0.1.2 Discuss how you would implement the following calculations, with a function, as they are not available in sklearn (this is a big part of HW4!)

0.1.3 Missing information for assessing coefficients:

- 95% CI
- Standard Error for β_0 and β_1
- P-value for test of H_0

0.1.4 Missing information for assessing the model:

- RSE , RSS , R^2

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd

from sklearn import linear_model
%matplotlib inline
```

In [2]:
```
#model: Y = 3X + 4
#size of training data and scale of random noise
pts=25
noisescale=.25
x=np.linspace(-50,50,num=pts)
B0=4
B1=3
yactual=B0+B1*x
np.random.seed(123) #for reproducible
```

```
#add noise scaled to 25% of range to data
yrand=yactual+noisescale*(yactual.max()-yactual.min())*np.random.normal(size=pts)
```

In [3]:
```
x
```

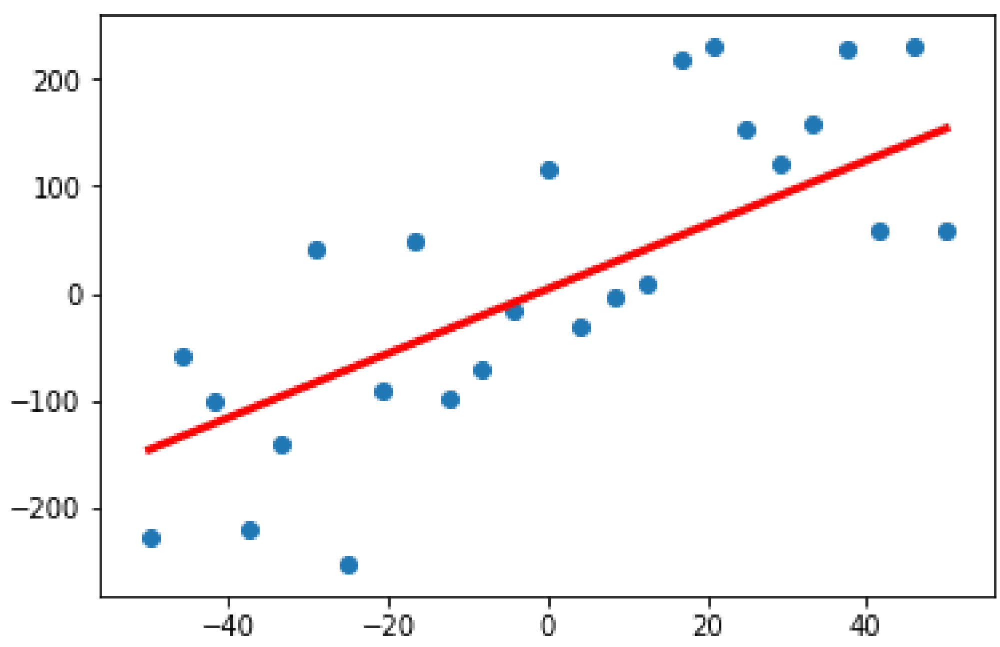
Out[3]:
```
array([-50.        , -45.83333333, -41.66666667, -37.5       ,
       -33.33333333, -29.16666667, -25.        , -20.83333333,
       -16.66666667, -12.5       ,  -8.33333333,  -4.16666667,
         0.        ,   4.16666667,   8.33333333,  12.5       ,
        16.66666667,  20.83333333,  25.        ,  29.16666667,
        33.33333333,  37.5       ,  41.66666667,  45.83333333,
        50.        ])
```

In [5]:
```
yrand
```

Out[5]:
```
array([-227.42229525,  -58.69909151,  -99.77661265, -221.47210354,
       -139.3950189 ,   40.35774028, -253.00094325,  -90.66844716,
         48.9452194 ,  -98.50553017,  -71.91646137,  -15.60317267,
        115.85422196,  -31.41764975,   -4.29864697,    8.92365433,
        219.4447562 ,  230.50895667,  154.30404234,  120.46397994,
        159.30264319,  228.30490211,   58.81245987,  229.68717836,
         59.95894992])
```

In [6]:
```
plt.plot(x,yactual,color='red',lw='3')
plt.scatter(x,yrand)
```

Out[6]:
```
<matplotlib.collections.PathCollection at 0x227b729bbe0>
```



In [16]:
```
x.reshape(-1,1)
```

Out[16]:
```
array([[-50.        ],
       [-45.83333333],
       [-41.66666667],
       [-37.5       ],
       [-33.33333333],
       [-29.16666667],
       [-25.        ],
       [-20.83333333],
       [-16.66666667],
       [-12.5       ],
       [ -8.33333333],
       [ -4.16666667],
       [  0.        ],
       [  4.16666667],
       [  8.33333333],
       [ 12.5       ],
       [ 16.66666667],
       [ 20.83333333],
       [ 25.        ],
       [ 29.16666667],
       [ 33.33333333],
       [ 37.5       ],
       [ 41.66666667],
       [ 45.83333333],
       [ 50.        ]])
```

In [15]:
```
x
```

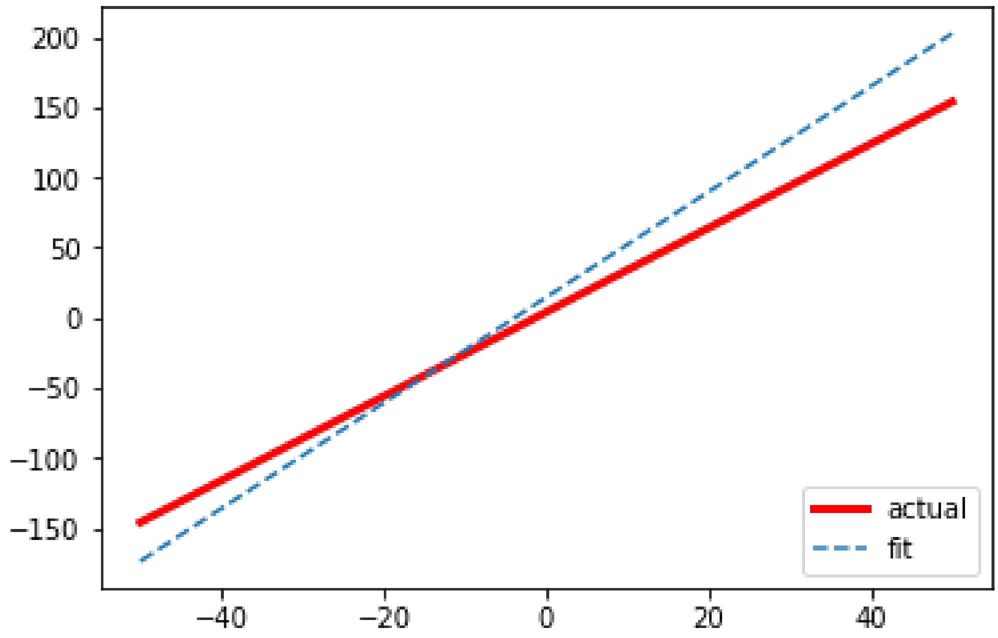
Out[15]:
```
array([-50.        , -45.83333333, -41.66666667, -37.5       ,
       -33.33333333, -29.16666667, -25.        , -20.83333333,
       -16.66666667, -12.5       ,  -8.33333333,  -4.16666667,
         0.        ,   4.16666667,   8.33333333,  12.5       ,
        16.66666667,  20.83333333,  25.        ,  29.16666667,
        33.33333333,  37.5       ,  41.66666667,  45.83333333,
        50.        ])
```

In [17]:
```
#EXPLAIN IN PLAIN LANGUAGE WHAT THIS LINE IS DOING!
regr=linear_model.LinearRegression()
# note that x.reshape(-1,1) is required because I must strictly
# feed regr.fit a 200x1 array , np.linspace returned a list of numbers
regr.fit(x.reshape(-1,1),yrand.reshape(-1,1))
print('B0, B1: ',regr.intercept_, regr.coef_[0])
```

```
B0, B1:  [14.50770926] [3.76217657]
```

In [19]:
```
plt.plot(x,yactual,color='red',lw='3',label='actual')
plt.plot(x,regr.predict(x.reshape(-1,1)),ls='--',label='fit')
plt.legend(loc='lower right')
```

Out[19]: <matplotlib.legend.Legend at 0x227b83296d8>



0.1.5 Take a few mins and see if you can

Useful plots to make after simple linear regression:

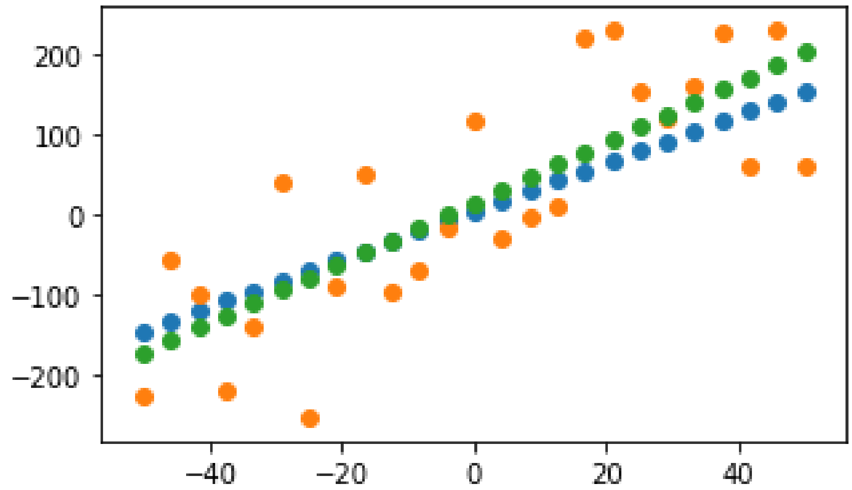
1) X vs Y (showing both training data, fit model, and result of predictionsw on test data (if you have any)

2) Y vs Y(hat): this is called a *parity plot*

3) X v s *residual* (Y - Y(hat))

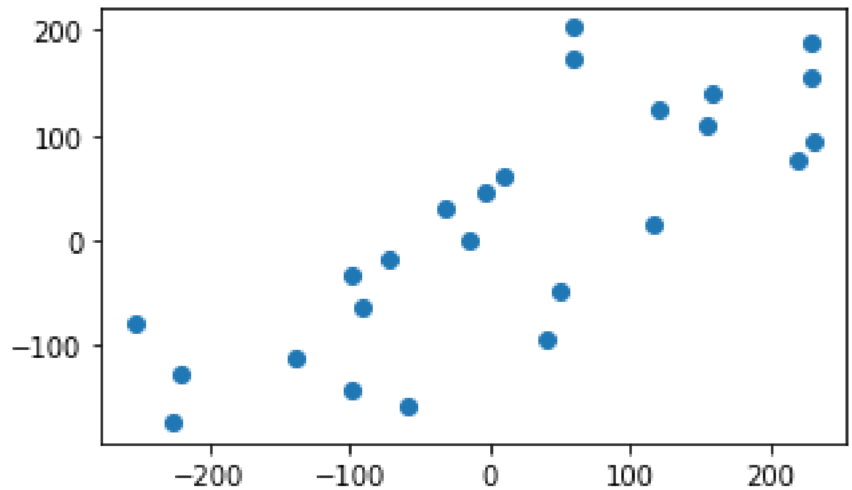
In [24]:
```
fig, ax = plt.subplots(figsize=(5, 3))
ax.scatter(x, yactual, label='actual')
ax.scatter(x, yrand, label='measured')
ax.scatter(x, regr.predict(x.reshape(-1,1)), label='predicted')
```

Out[24]: <matplotlib.collections.PathCollection at 0x227b853e5c0>



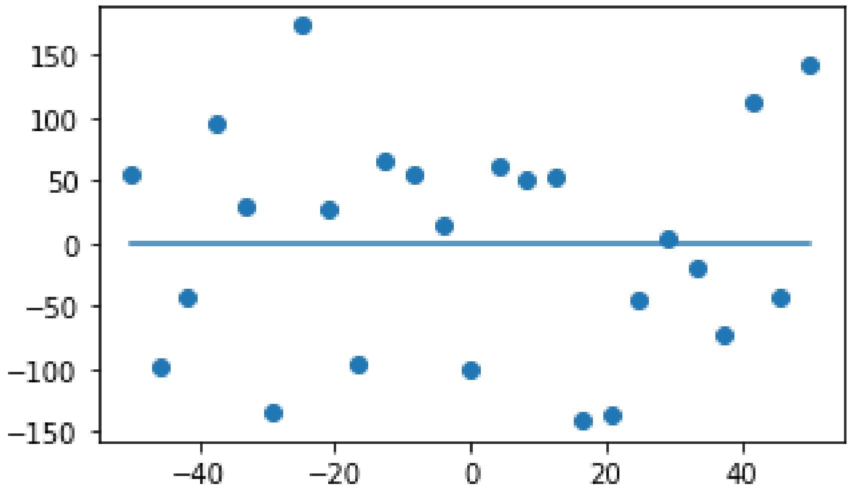

```
In [34]: fig, ax = plt.subplots(figsize=(5, 3))
         ax.scatter(yrand, regr.predict(x.reshape(-1,1)), label='parity')
```

```
Out[34]: <matplotlib.collections.PathCollection at 0x227b88a1908>
```




```
In [37]: fig, ax = plt.subplots(figsize=(5, 3))
         ax.scatter(x, regr.predict(x.reshape(-1,1)) - yrand)
         ax.plot(x, 0*x)
```

```
Out[37]: [<matplotlib.lines.Line2D at 0x227b8554b00>]
```



0.1.6 Multiple linear regression

In this 2nd example, we generate model based on the idea that the *PCE* of a candidate organic photovoltaic can be modeled as a contribution of the molecule's *mass*, *VOC* and E_{LUMO} values: $PCE = \beta_0 + \beta_1 * mass + \beta_2 * VOC + \beta_3 * E_{LUMO}$

The extension from simple to multiple linear regression is trivial - can you figure it out with your partner or at your table?!

```
In [38]: harvard=pd.read_csv('https://raw.githubusercontent.com/UWDIRECT/UWDIRECT.github.io/mas
         # you need to complete these lines
         # (but first you might refresh yourself on what is contained in harvard

         # keep the same variable names -
         # regr2=STUFF
         # regr2.fit(STUFF)
         # once your model is trained, can you make a parity plot: plot actual PCE data on x v
         # trained PCE data on y. Also plot the line of parity so your eye can follow how good
         # your predictions are doing....
```

```
In [ ]: #model: Y = 3X + 4
        #size of training data and scale of random noise
```

```
In [44]: def regression(points=25, x_range=[-50,50], coefs=[4, 3], noisescale=0.25):
             pts=25
             noisescale=.25
             x=np.linspace(x_range[0],x_range[1],num=points)
             B0=coefs[0]
             B1=coefs[1]
             yactual=B0+B1*x
             #np.random.seed(123) #for reproducible
```

```
        #add noise scaled to 25% of range to data
        yrand=yactual+noisescale*(yactual.max()-yactual.min())*np.random.normal(size=poin

        #EXPLAIN IN PLAIN LANGUAGE WHAT THIS LINE IS DOING!
        regr=linear_model.LinearRegression()
        # note that x.reshape(-1,1) is required because I must strictly
        # feed regr.fit a 200x1 array , np.linspace returned a list of numbers
        regr.fit(x.reshape(-1,1),yrand.reshape(-1,1))
        return regr.intercept_[0], regr.coef_[0][0]
```

```
In [45]: repeats = 1000
         B0 = [0]*repeats
         B1 = [0]*repeats
         for i in range(repeats):
             B0[i], B1[i] = regression(points=25, noisescale=0.25)
```

```
In [57]: repeats = 1000
         noisescale = 0.25
         B0 = [0]*repeats
         B1 = [0]*repeats
         for i in range(repeats):
             B0[i], B1[i] = regression(points=25, noisescale=noisescale)
         print('95% CI Intercept: {} - {}'.format(np.round(np.percentile(np.array(B0), 5), 2),
         print('95% CI Intercept: {} - {}'.format(np.round(np.percentile(np.array(B1), 5), 2),
```

```
95% CI Intercept: -19.17 - 28.09
95% CI Intercept: 2.22 - 3.73
```

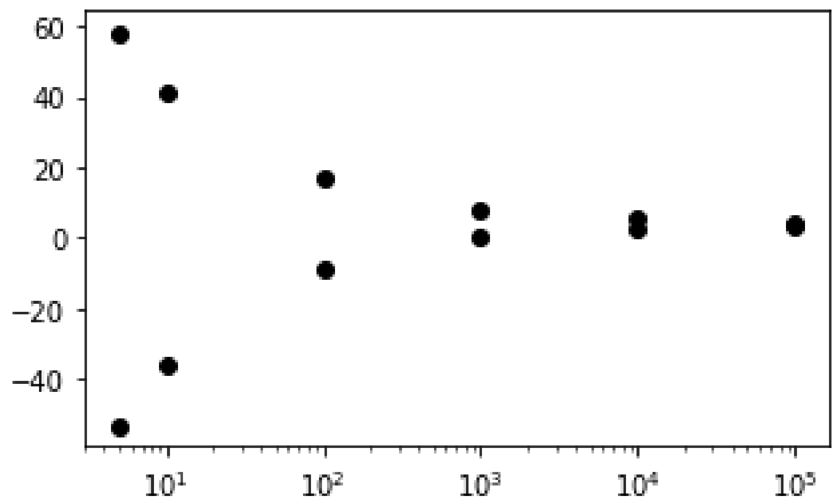
```
In [84]: def regression_cis(points, noisescale, repeats):
             B0 = [0]*repeats
             B1 = [0]*repeats
             for i in range(repeats):
                 B0[i], B1[i] = regression(points=points, noisescale=noisescale)
             print('95% CI Intercept: {} - {}'.format(np.round(np.percentile(np.array(B0), 5),
             print('95% CI Slope: {} - {}'.format(np.round(np.percentile(np.array(B1), 5), 2),
             return [np.percentile(np.array(B0), 5), np.percentile(np.array(B0), 95)], [np.perc
```

```
In [85]: B0cilo = []
         B0cihi = []
         B1cilo = []
         B1cihi = []
         points = [5, 10, 100, 1000, 10000, 100000]
         for i in points:
             B0ci0, B1ci0 = regression_cis(i, noisescale, 1000)
             B0cilo.append(B0ci0[0])
             B0cihi.append(B0ci0[1])
             B1cilo.append(B1ci0[0])
             B1cihi.append(B1ci0[1])
```

```
fig, ax = plt.subplots(figsize=(5, 3))
ax.scatter(points, B0cilo, color='k')
ax.scatter(points, B0cihi, color='k')
plt.semilogx()
```

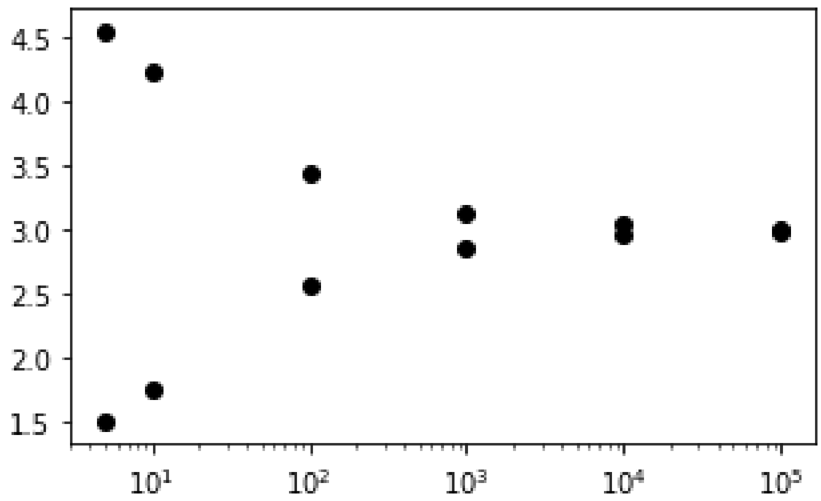
```
95% CI Intercept: -53.26 - 58.09
95% CI Slope: 1.51 - 4.56
95% CI Intercept: -35.92 - 41.17
95% CI Slope: 1.76 - 4.24
95% CI Intercept: -8.53 - 16.75
95% CI Slope: 2.57 - 3.44
95% CI Intercept: 0.05 - 7.91
95% CI Slope: 2.87 - 3.13
95% CI Intercept: 2.73 - 5.3
95% CI Slope: 2.96 - 3.04
95% CI Intercept: 3.61 - 4.35
95% CI Slope: 2.99 - 3.01
```

Out[85]: []



In [86]:
```
fig, ax = plt.subplots(figsize=(5, 3))
ax.scatter(points, B1cilo, color='k')
ax.scatter(points, B1cihi, color='k')
plt.semilogx()
```

Out[86]: []



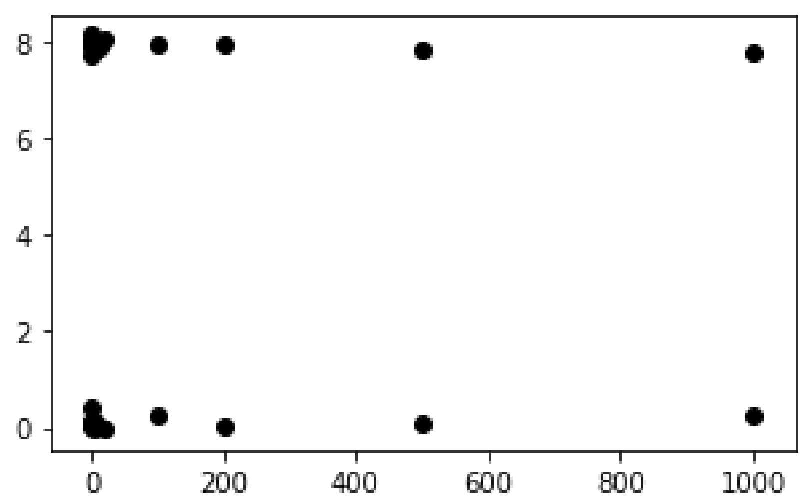

```
In [97]: B0cilo = []
         B0cihi = []
         B1cilo = []
         B1cihi = []
         points = [0.01, 0.05, 0.1, 0.25, 0.5, 1, 2, 5, 10, 20, 100, 200, 500, 1000]
         for noise in points:
             B0ci0, B1ci0 = regression_cis(1000, noise, 1000)
             B0cilo.append(B0ci0[0])
             B0cihi.append(B0ci0[1])
             B1cilo.append(B1ci0[0])
             B1cihi.append(B1ci0[1])

         fig, ax = plt.subplots(figsize=(5, 3))
         ax.scatter(points, B0cilo, color='k')
         ax.scatter(points, B0cihi, color='k')
```

```
95% CI Intercept: 0.16 - 7.7
95% CI Slope: 2.86 - 3.14
95% CI Intercept: 0.04 - 7.99
95% CI Slope: 2.87 - 3.12
95% CI Intercept: 0.08 - 7.97
95% CI Slope: 2.86 - 3.13
95% CI Intercept: 0.41 - 7.87
95% CI Slope: 2.86 - 3.13
95% CI Intercept: 0.02 - 8.15
95% CI Slope: 2.87 - 3.13
95% CI Intercept: 0.11 - 7.97
95% CI Slope: 2.87 - 3.13
95% CI Intercept: 0.15 - 8.02
```

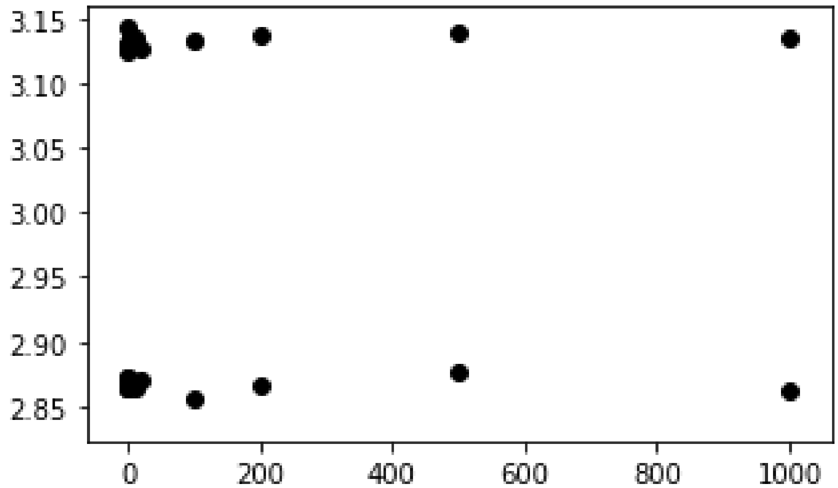
```
95% CI Slope: 2.87 - 3.14
95% CI Intercept: -0.03 - 8.02
95% CI Slope: 2.87 - 3.13
95% CI Intercept: 0.02 - 7.9
95% CI Slope: 2.86 - 3.14
95% CI Intercept: -0.01 - 8.08
95% CI Slope: 2.87 - 3.13
95% CI Intercept: 0.27 - 7.94
95% CI Slope: 2.86 - 3.13
95% CI Intercept: 0.03 - 7.95
95% CI Slope: 2.87 - 3.14
95% CI Intercept: 0.08 - 7.83
95% CI Slope: 2.88 - 3.14
95% CI Intercept: 0.26 - 7.77
95% CI Slope: 2.86 - 3.14
```

Out[97]: <matplotlib.collections.PathCollection at 0x227b9271390>



In [98]:
```
fig, ax = plt.subplots(figsize=(5, 3))
ax.scatter(points, B1cilo, color='k')
ax.scatter(points, B1cihi, color='k')
```

Out[98]: <matplotlib.collections.PathCollection at 0x227b95a0a20>



In [ ]: