HOMEWORK 1 - Due 9/6/2012

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9/6/12 Thursday

Contents

1 Signup for an account at gitHub.

Print your username here: zhongnanxu (note, I've changed it from my previous 'xuzho' one for consistency)

Set yourself up to watch https://github.com/jkitchin/dft-course and https://github.com/jkitchin/dft-book.

2 Read Chapter 1 in the text book.

You do not need to write anything. Just do it.

3 Read Section 5 (Molecules) in dft-book.

As part of this assignment, please turn in a pdf copy of dft-book that has been annotated by sticky notes using Adobe Acrobat Reader (you should be able to type Ctrl-6 to get a sticky note while the pdf is open, and then you can move it where you want and type text in it.). Please note any typos, places that are confusing, etc...

Please see pdf file in the hw-1 folder

4 Data fitting.

Fit a cubic polynomial to this set of data and estimate the lattice constant that minimizes the total energy. Prepare a figure that shows the data, your fit and your estimated minimum. Hints: `numpy.polyfit`, `numpy.polyder`, `numpy.roots`, `numpy.linspace`, `numpy.polyval` will all help you do this easily.

lattice constant (Å)	Total Energy (eV)
3.5	-3.649238
3.55	-3.696204
3.6	-3.719946
3.65	-3.723951
3.7	-3.711284
3.75	-3.68426

Code

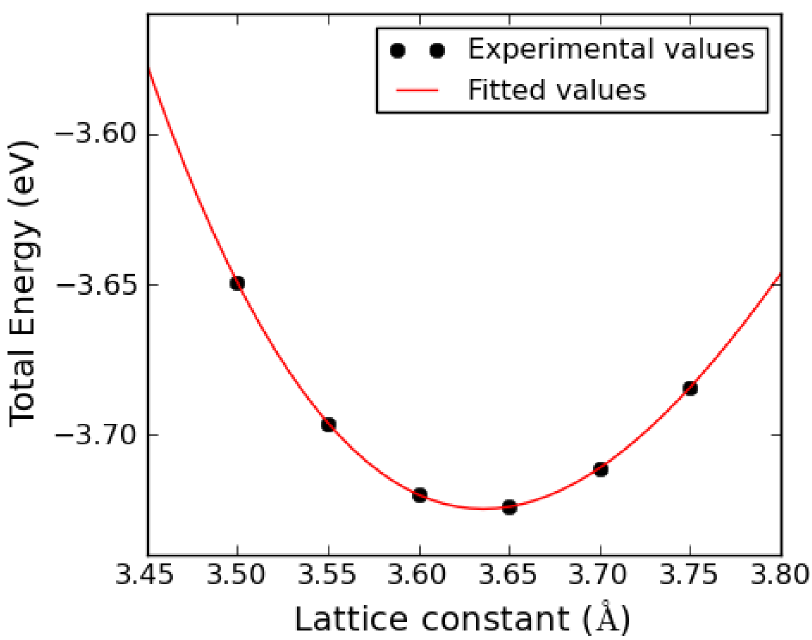
```
import numpy as np
import matplotlib.pyplot as plt

lats, energies = zip(*table)
coeffs = np.polyfit(lats, energies, 3)
ders = np.polyder(coeffs)
roots = np.roots(ders)
# We now need to see what the roots are and pick the sensible one
print 'The two roots are {0:1.3f} and {1:1.3f}'.format(roots[0], roots[1])
print 'Therefore, {0:1.3f} is the minimum lattice constant'.format(roots[1])
lats_func = np.linspace(3.45, 3.80)
energies_func = np.polyval(coeffs, lats_func)
```

```
fig = plt.figure(1, (5, 4))
ax = fig.add_subplot(111)
ax.plot(lats, energies, marker='o', linestyle='None', color='k',
        label='Experimental values')
ax.plot(lats_func, energies_func, marker='None', linestyle='-', color='r',
        label='Fitted values')
ax.set_xlabel('Lattice constant ($\AA$)', size='large')
ax.set_ylabel('Total Energy (eV)', size='large')
ax.legend(prop={'size':'medium'})
fig.tight_layout()
plt.show()
```

Output

```
The two roots are 4.233 and 3.636
Therefore, 3.636 is the minimum lattice constant
```



5 Nonlinear algebra

Solve this equation: $\sin(x^2) = 0.5$ for x. Prepare a plot of the function and show where your solution is. Hint: `scipy.optimize.fsolve`

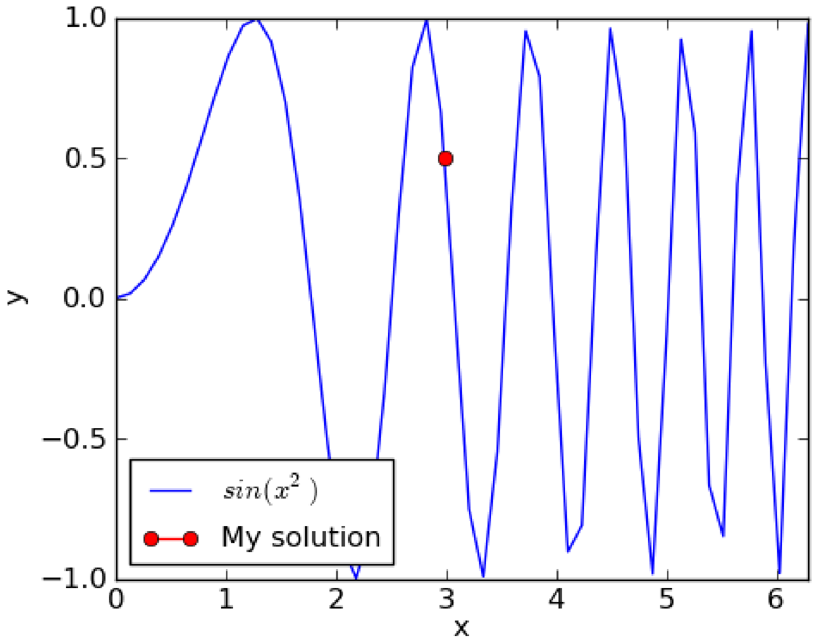
Code

```
import numpy as np
from scipy.optimize import fsolve
import matplotlib.pyplot as plt

def func(x):
    return np.sin(x**2) - 0.5
print 'The answer is {0:1.3f}'.format(fsolve(func, np.pi)[0])
fig = plt.figure(1, (5, 4))
ax = fig.add_subplot(111)
x = np.linspace(0, 2 * np.pi)
y = func(x) + 0.5
ax.plot(x, y, marker='None', color='b', label='$sin(x^2)$')
ax.plot(2.983, np.sin(2.983**2), marker='o', color='r', label='My solution')
ax.set_xlabel('x')
ax.set_ylabel('y')
ax.set_xlim((0, 2 * np.pi))
ax.legend(prop={'size':'medium'}, loc=3)
fig.tight_layout()
plt.show()
```

Output

```
The answer is 2.983
```



6 Linear algebra

Solve these equations using python and linear algebra:

$$a0 - 3a1 + 9a2 - 27a3 = -2 \quad (1)$$
$$a0 - a1 + a2 - a3 = 2 \quad (2)$$
$$a0 + a1 + a2 + a3 = 5 \quad (3)$$
$$a0 + 2a1 + 4a2 + 8a3 = 1 \quad (4)$$

Use linear algebra to verify your solution. Hint: see `numpy.linalg`, `numpy.dot`.

Code

```
import numpy as np
# This can be solved with matrix algebra, Ax = B
a = np.array([[1, -3, 9, -27],
             [1, -1, 1, -1],
             [1, 1, 1, 1],
```

```
             [1, 2, 4, 8]])
b = np.array([-2, 2, 5, 1])
x = np.linalg.solve(a, b)
print 'The answer is'
print 'a0={0:1.3f}'.format(x[0])
print 'a1={0:1.3f}'.format(x[1])
print 'a2={0:1.3f}'.format(x[2])
print 'a3={0:1.3f}'.format(x[3])
# Check that the solution is correct by performing a
# A dot x operation
print np.dot(a, x)
```

Output

```
The answer is
a0=4.650
a1=1.842
a2=-1.150
a3=-0.342
[-2.  2.  5.  1.]
```