VQE with Linear and Exponential Extrap (June 16)-Copy1

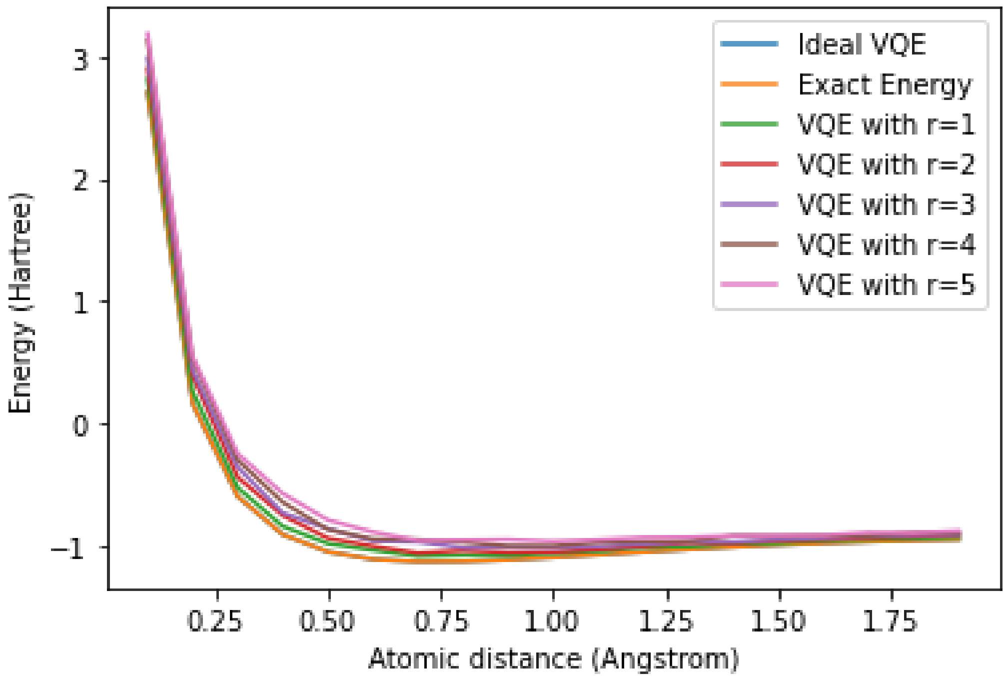
June 19, 2020

1 Does Noise Amplification affect VQE Computations?

For Extrapolation to be useful, this condition has to be met.

2 VQE with different noise scalings

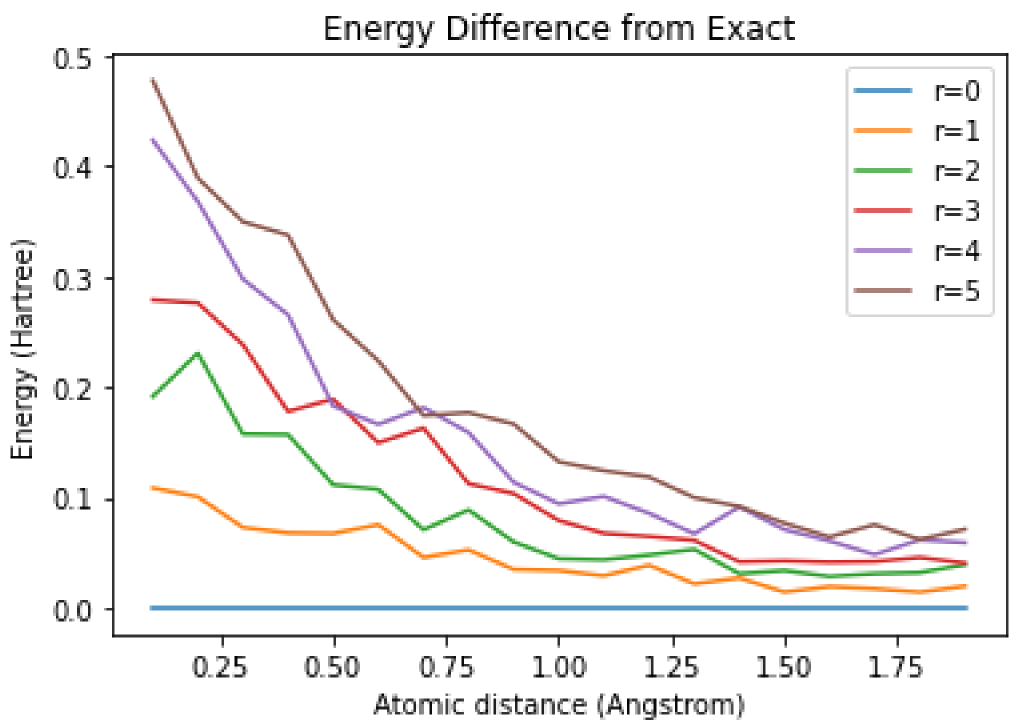
[29]:
```
# plotting the data
plt.plot(distances, vqe_ideal_energy, label="Ideal VQE")
plt.plot(distances, exact_energies, label="Exact Energy")

plt.plot(distances, vqe_energies[0], label="VQE with r=1")
plt.plot(distances, vqe_energies[1], label="VQE with r=2")
plt.plot(distances, vqe_energies[2], label="VQE with r=3")
plt.plot(distances, vqe_energies[3], label="VQE with r=4")
plt.plot(distances, vqe_energies[4], label="VQE with r=5")
plt.xlabel('Atomic distance (Angstrom)')
plt.ylabel('Energy (Hartree)')
plt.legend()
plt.show()
```



[30]:

```
energy_difference= []
for i in range(6):
    energy_difference.append([])

for i in range(6):
    if (i ==0):
        for k in range(len(vqe_ideal_energy)):
            energy_difference[i] = energy_difference[i] + [vqe_ideal_energy[k] -
 ↪exact_energies[k]]
    else:
        for k in range(len(vqe_ideal_energy)):
            energy_difference[i] = energy_difference[i] + [vqe_energies[i-1][k]
 ↪- exact_energies[k]]


plt.plot(distances, energy_difference[0], label="r=0")
plt.plot(distances, energy_difference[1], label="r=1")
plt.plot(distances, energy_difference[2], label="r=2")
plt.plot(distances, energy_difference[3], label="r=3")
plt.plot(distances, energy_difference[4], label="r=4")
plt.plot(distances, energy_difference[5], label="r=5")
```

```
plt.xlabel('Atomic distance (Angstrom)')
plt.ylabel('Energy (Hartree)')
plt.title('Energy Difference from Exact')
plt.legend()
plt.show()
```



3 Analysis

The graph suggests that if we scale the depolarizing error higher and higher, our results tend to go away from the exact energy. So noise amplification diverges VQE estimate from actual answer.

4 To do next

Extrapolate

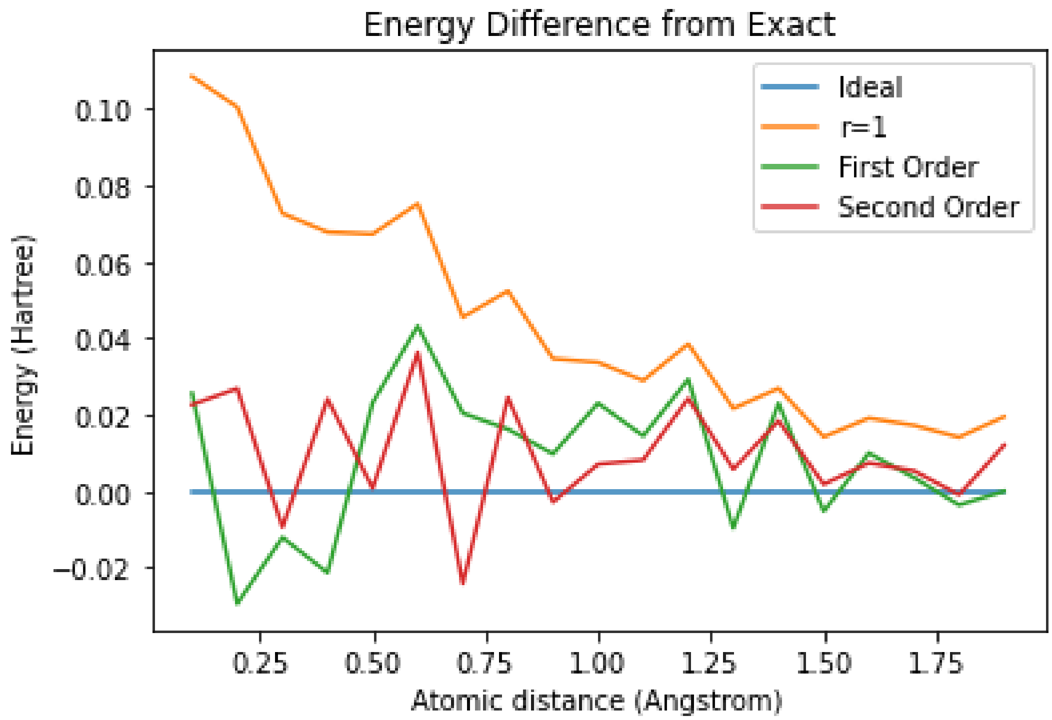
5 Linear Extrapolation Using Curve Fitting

Instead of using the equations-method (which I used earlier and messed up) as shown in section 3 in supplemental materials of Temme Paperm, here I use a simple curve fitting technique.

How the curve fitting technique works is shown later in this document.

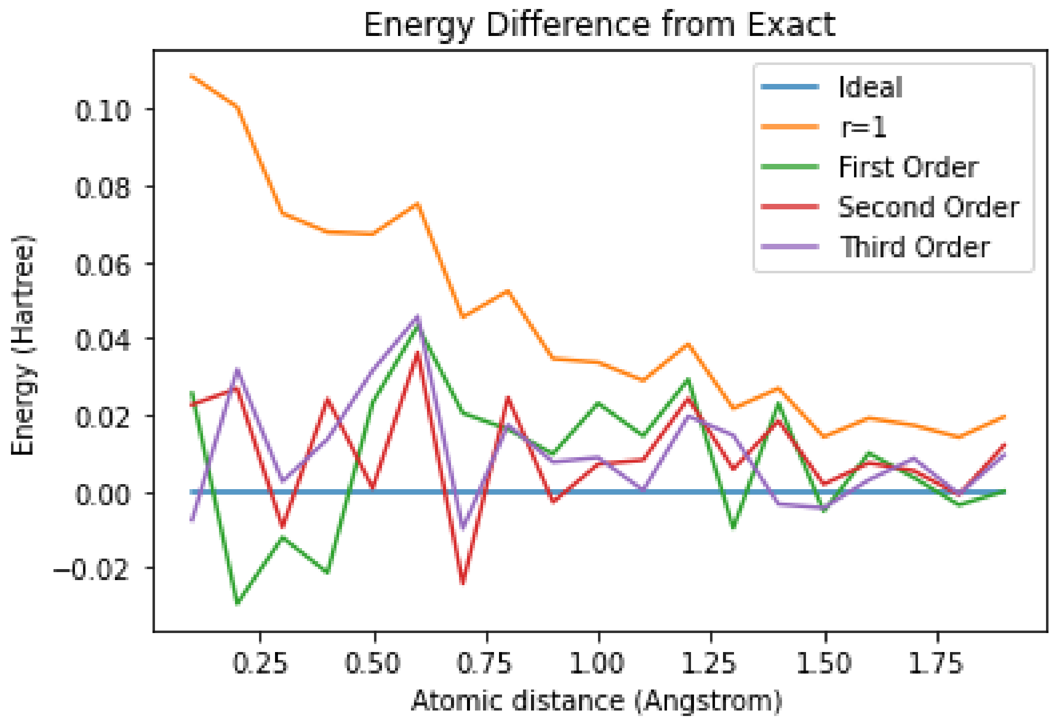
[31]:

```
from scipy.optimize import curve_fit
# extrapolating to 4 orders the entire thing through curve fitting
orders = []
orders_diff =[]
plot = []
for i in range(2,6):
    #building up orders through curve fitting
    some_order = []
    for k in range(len(vqe_ideal_energy)):
        plot=[]
        x = np.array([])
        y = np.array([])
        for c in range(i):
            x = np.append(x, [c+1])
            y = np.append(y, [vqe_energies[c][k]])
        plot.append(x)
        plot.append(y)
        def fit_func(x, a, b):
            return a*x + b
        params = curve_fit(fit_func, x, y)
        [a, b] = params[0]
        plot.append([a, b])
        some_order.append(params[0][1])
    orders.append(some_order)
#differences from exact
for order in orders:
    some_diff = []
    for k in range(len(vqe_ideal_energy)):
        some_diff = some_diff + [order[k] - exact_energies[k]]
    orders_diff.append(some_diff)
#plotting energy differences
plt.plot(distances, energy_difference[0], label="Ideal")
plt.plot(distances, energy_difference[1], label="r=1")
plt.plot(distances, orders_diff[0], label="First Order", color= 'tab:green')
plt.plot(distances, orders_diff[1], label="Second Order", color= 'tab:red')
#plt.plot(distances, orders_diff[2], label="Third Order")
#plt.plot(distances, orders_diff[3], label="Fourth Order")


plt.xlabel('Atomic distance (Angstrom)')
plt.ylabel('Energy (Hartree)')
plt.title('Energy Difference from Exact')
plt.legend()
plt.show()
```

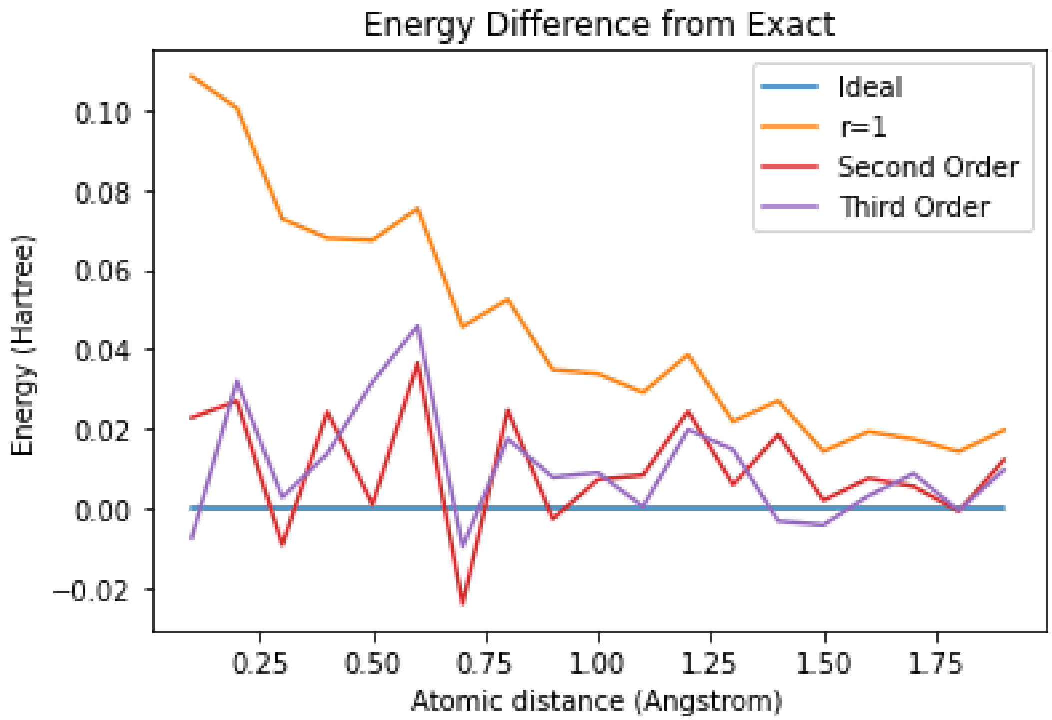


5.1 Adding in Third Order

[32]:
```
plt.plot(distances, energy_difference[0], label="Ideal")
plt.plot(distances, energy_difference[1], label="r=1")
plt.plot(distances, orders_diff[0], label="First Order", color= 'tab:green')
plt.plot(distances, orders_diff[1], label="Second Order", color= 'tab:red')
plt.plot(distances, orders_diff[2], label="Third Order", color = 'tab:purple')
#plt.plot(distances, orders_diff[3], label="Fourth Order")


plt.xlabel('Atomic distance (Angstrom)')
plt.ylabel('Energy (Hartree)')
plt.title('Energy Difference from Exact')
plt.legend()
plt.show()
```

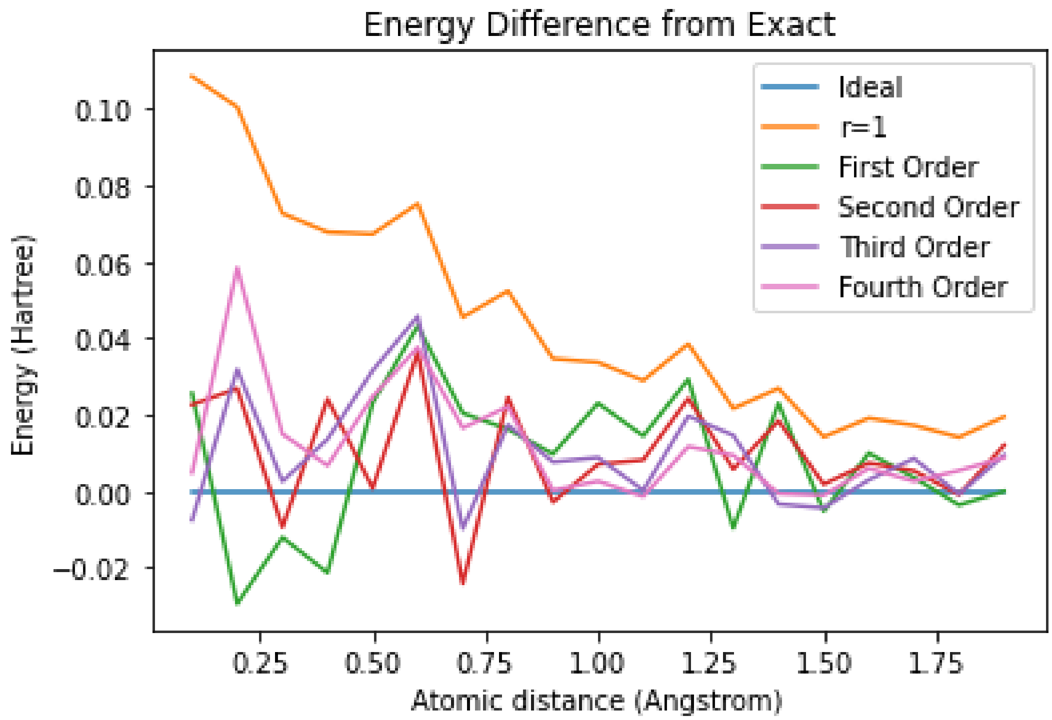


[33]:
```
plt.plot(distances, energy_difference[0], label="Ideal")
plt.plot(distances, energy_difference[1], label="r=1")
#plt.plot(distances, orders_diff[0], label="First Order", color= 'tab:green')
plt.plot(distances, orders_diff[1], label="Second Order", color= 'tab:red')
plt.plot(distances, orders_diff[2], label="Third Order", color = 'tab:purple')
#plt.plot(distances, orders_diff[3], label="Fourth Order")


plt.xlabel('Atomic distance (Angstrom)')
plt.ylabel('Energy (Hartree)')
plt.title('Energy Difference from Exact')
plt.legend()
plt.show()
```



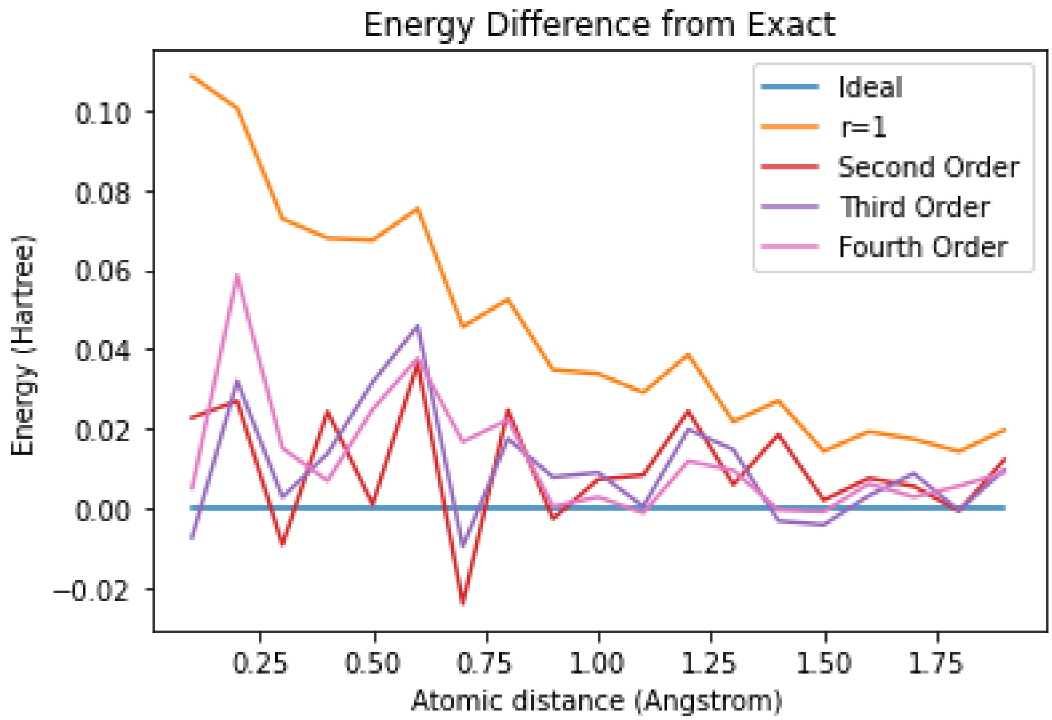
5.2 Fourth Order

[34]:
```
plt.plot(distances, energy_difference[0], label="Ideal")
plt.plot(distances, energy_difference[1], label="r=1")
plt.plot(distances, orders_diff[0], label="First Order", color= 'tab:green')
plt.plot(distances, orders_diff[1], label="Second Order", color= 'tab:red')
plt.plot(distances, orders_diff[2], label="Third Order", color = 'tab:purple')
plt.plot(distances, orders_diff[3], label="Fourth Order", color = 'tab:pink')


plt.xlabel('Atomic distance (Angstrom)')
plt.ylabel('Energy (Hartree)')
plt.title('Energy Difference from Exact')
plt.legend()
plt.show()
```

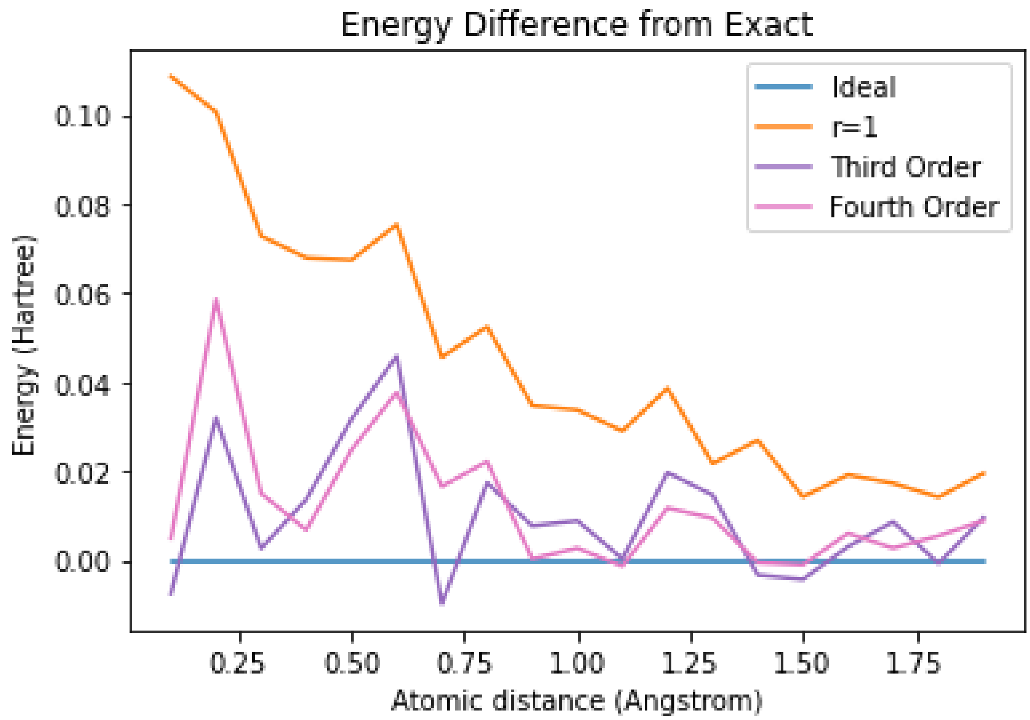


[35]:

```
plt.plot(distances, energy_difference[0], label="Ideal")
plt.plot(distances, energy_difference[1], label="r=1")
#plt.plot(distances, orders_diff[0], label="First Order", color= 'tab:green')
plt.plot(distances, orders_diff[1], label="Second Order", color= 'tab:red')
plt.plot(distances, orders_diff[2], label="Third Order", color = 'tab:purple')
plt.plot(distances, orders_diff[3], label="Fourth Order", color = 'tab:pink')


plt.xlabel('Atomic distance (Angstrom)')
plt.ylabel('Energy (Hartree)')
plt.title('Energy Difference from Exact')
plt.legend()
plt.show()
```



[36]:
```
plt.plot(distances, energy_difference[0], label="Ideal")
plt.plot(distances, energy_difference[1], label="r=1")
#plt.plot(distances, orders_diff[0], label="First Order", color= 'tab:green')
#plt.plot(distances, orders_diff[1], label="Second Order", color= 'tab:red')
plt.plot(distances, orders_diff[2], label="Third Order", color = 'tab:purple')
plt.plot(distances, orders_diff[3], label="Fourth Order", color = 'tab:pink')


plt.xlabel('Atomic distance (Angstrom)')
plt.ylabel('Energy (Hartree)')
plt.title('Energy Difference from Exact')
plt.legend()
plt.show()
```



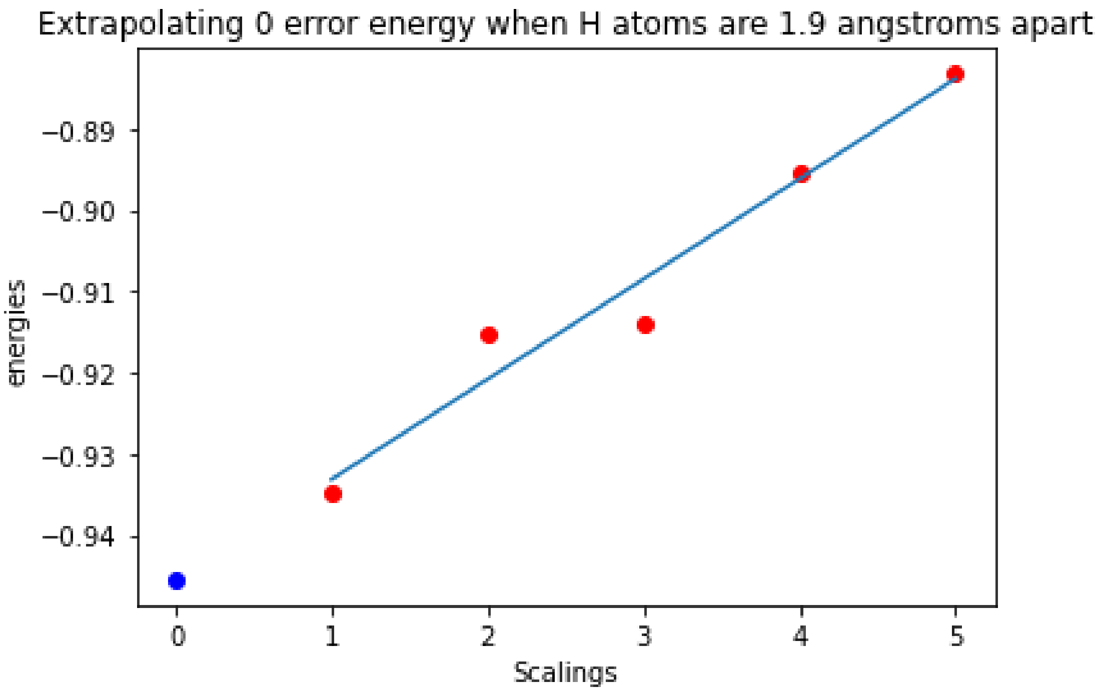
6 How it Works?

Consider the Graph below titled, "Extrapolating 0 error energy when H atoms are 1.9 angstroms apart." The red dots are the calculated energies when we scale by some factors. Those factors are labeled as "scalings" and this is done by increasing the error probabilities by some amount.

Using a SciPy package, we try to fit a line through those points using least squares. From that line, we extrapolate or extract the zero error solution i.e. if line is y= f(x), then we take out y(0).

Note: I can't connect the line to the blue point(zero error solution). But the blue point does sit on the line

[37]:
```
plt.plot(plot[0], plot[1], 'ro')
plt.plot(0, orders[3][18], 'bo')
plt.plot(x, plot[2][0]*x + plot[2][1])
plt.xlabel('Scalings')
plt.ylabel('energies')
plt.title('Extrapolating 0 error energy when H atoms are 1.9 angstroms apart')
plt.show()
```



6.1 Orders of Extrapolation

First Order: Fitting a line through 2 red points (r=1 and r=2)

Second Order: Fitting a line through 3 red points (r=1, r=2, r=3)

and on and on. In the graph above, we are performing a 4th order extrapolation!!

The assumption is that the more red points you have, the better the zero error solution (blue point).

7 Exponential Extrapolation

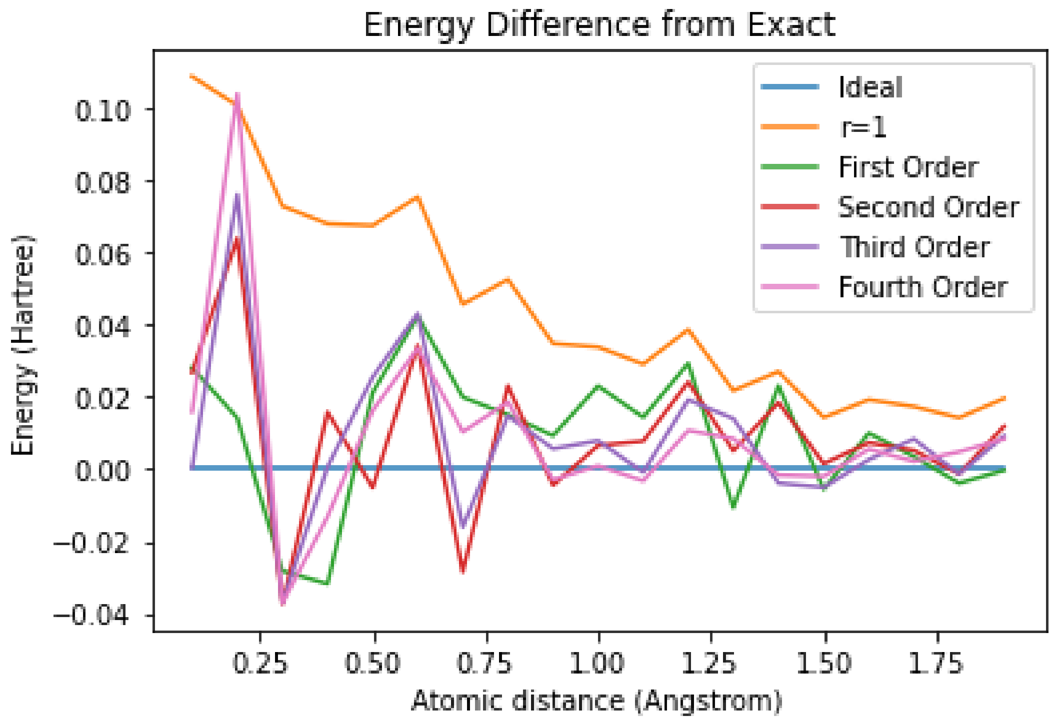
Instead of trying to fit a line through the points, lets try fitting an exponential curve of the form

$$a * e^{bx}$$

.

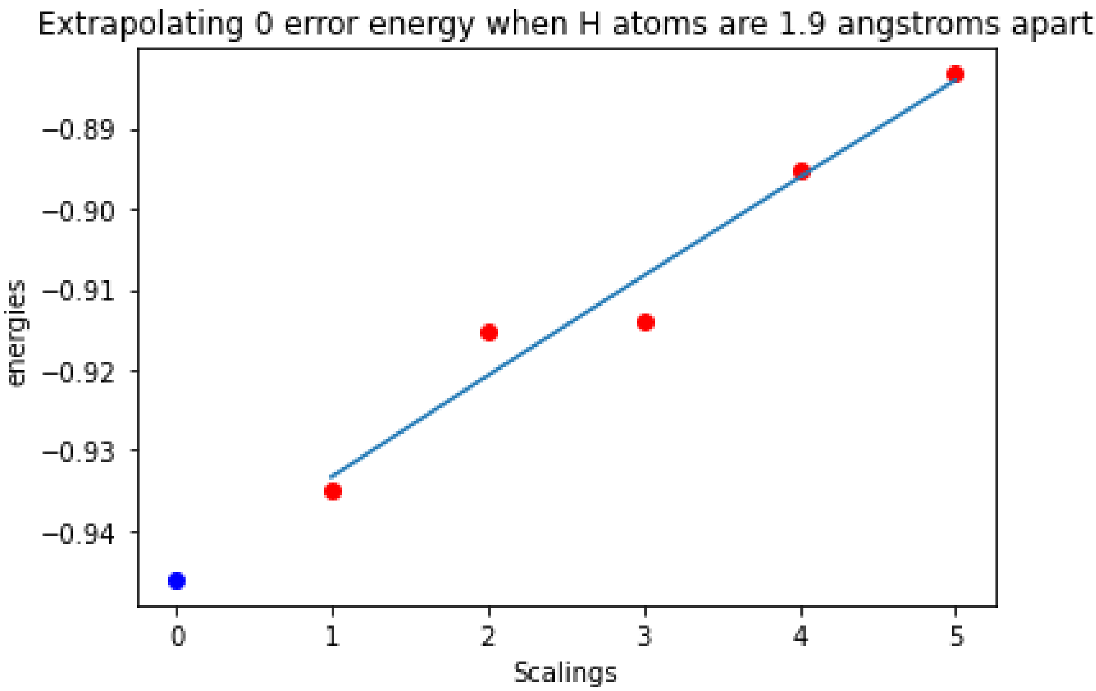
[38]:
```
# extrapolating to 4 orders the entire thing through curve fitting
ex_orders = []
ex_orders_diff =[]
ploty = []
for i in range(2,6):
    #building up orders through curve fitting
    some_order = []
    for k in range(len(vqe_ideal_energy)):
        ploty=[]
```

```
        x = np.array([])
        y = np.array([])
        for c in range(i):
            x = np.append(x, [c+1])
            y = np.append(y, [vqe_energies[c][k]])
        ploty.append(x)
        ploty.append(y)
        def fit_func(x, a, b):
            return a * np.exp(b * x)
        params = curve_fit(fit_func, x, y)
        [a, b] = params[0]
        ploty.append([a, b])
        some_order.append(params[0][0])
    ex_orders.append(some_order)
#differences from exact
for order in ex_orders:
    some_diff = []
    for k in range(len(vqe_ideal_energy)):
        some_diff = some_diff + [order[k] - exact_energies[k]]
    ex_orders_diff.append(some_diff)
#plotting energy differences
plt.plot(distances, energy_difference[0], label="Ideal")
plt.plot(distances, energy_difference[1], label="r=1")
plt.plot(distances, ex_orders_diff[0], label="First Order", color= 'tab:green')
plt.plot(distances, ex_orders_diff[1], label="Second Order", color= 'tab:red')
plt.plot(distances, ex_orders_diff[2], label="Third Order", color = 'tab:purple')
plt.plot(distances, ex_orders_diff[3], label="Fourth Order", color = 'tab:pink')


plt.xlabel('Atomic distance (Angstrom)')
plt.ylabel('Energy (Hartree)')
plt.title('Energy Difference from Exact')
plt.legend()
plt.show()
```



[39]:
```
plt.plot(ploty[0], ploty[1], 'ro')
plt.plot(0, ex_orders[3][18], 'bo')
a = ploty[2][0]
b= ploty[2][1]
print(a)
print(b)
plt.plot(x, a*np.exp(b*x))
plt.xlabel('Scalings')
plt.ylabel('energies')
plt.title('Extrapolating 0 error energy when H atoms are 1.9 angstroms apart')
plt.show()
```

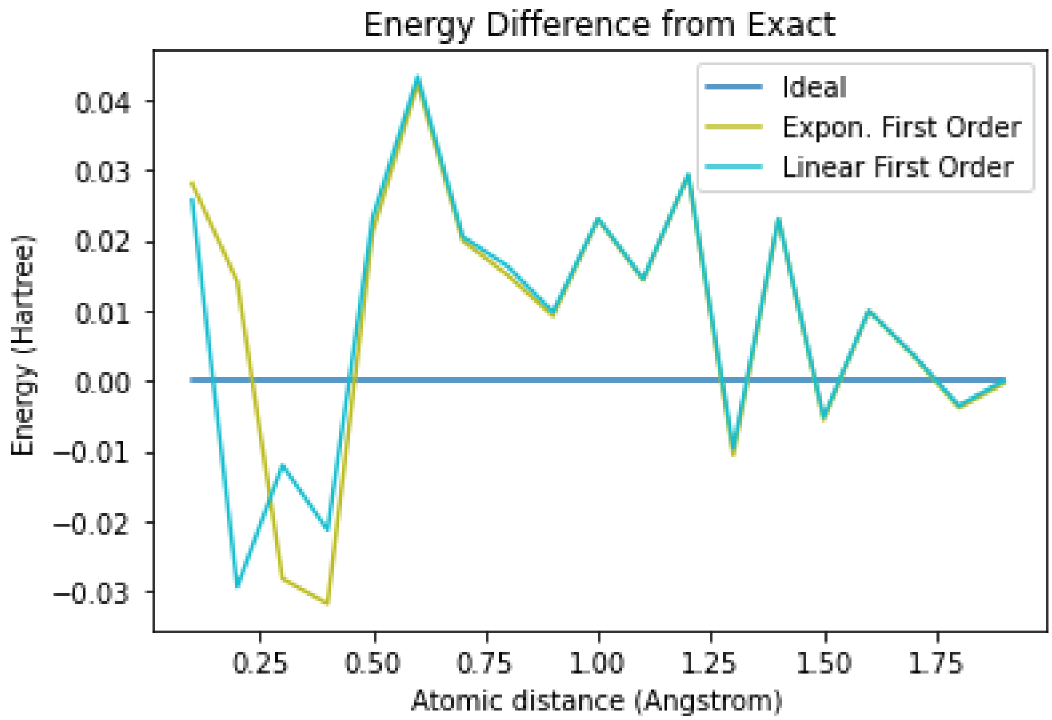
```
-0.9460324410809242
-0.013554953170051554
```



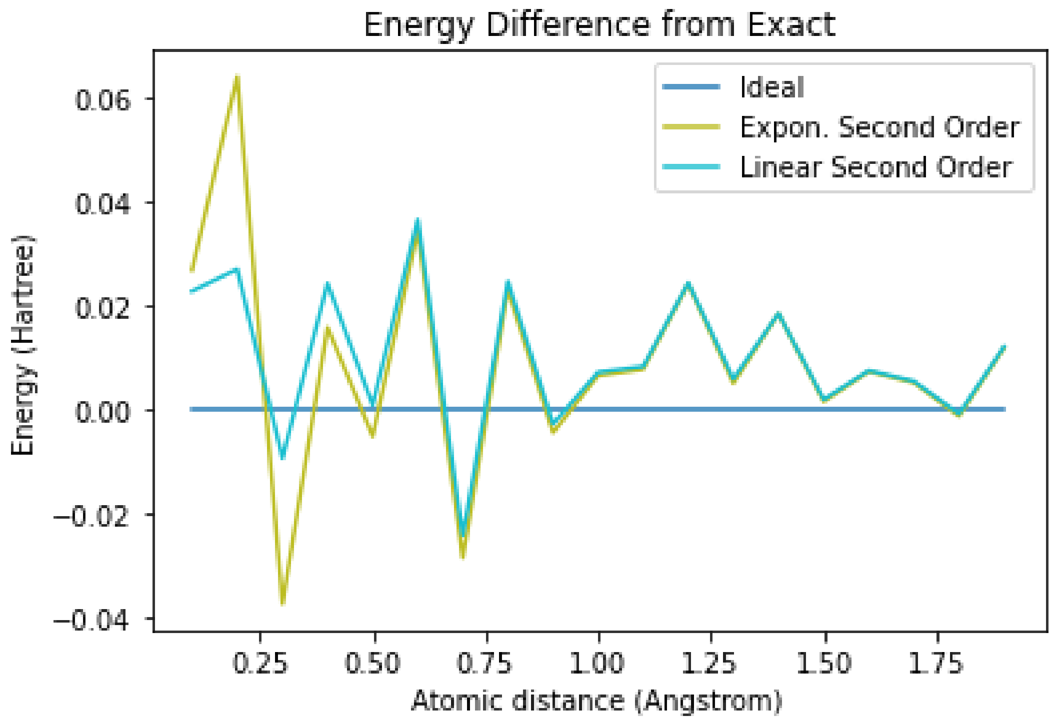
Should look like an exponential curve but the red dots are such that the curve fit package makes the exponential curve look like a line.

8 Comparing Linear Vs Extrapolation Results

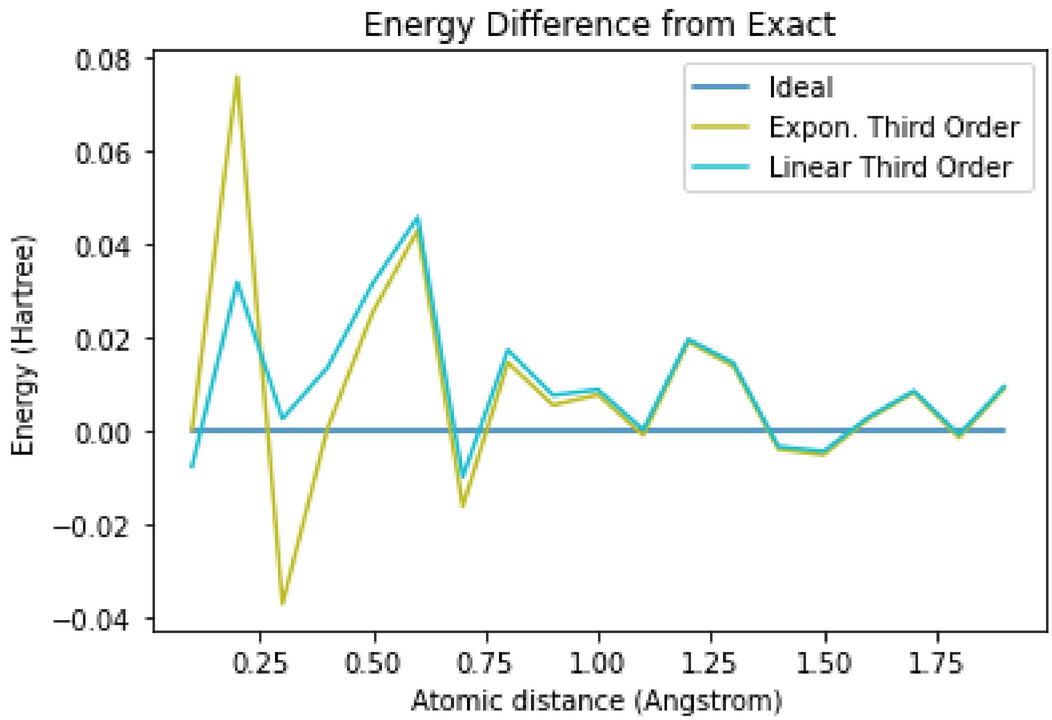
[40]:
```
plt.plot(distances, energy_difference[0], label="Ideal")
plt.plot(distances, ex_orders_diff[0], label="Expon. First Order", color= 'tab:
 ↪olive')
plt.plot(distances, orders_diff[0], label="Linear First Order", color= 'tab:
 ↪cyan')

plt.xlabel('Atomic distance (Angstrom)')
plt.ylabel('Energy (Hartree)')
plt.title('Energy Difference from Exact')
plt.legend()
plt.show()
```



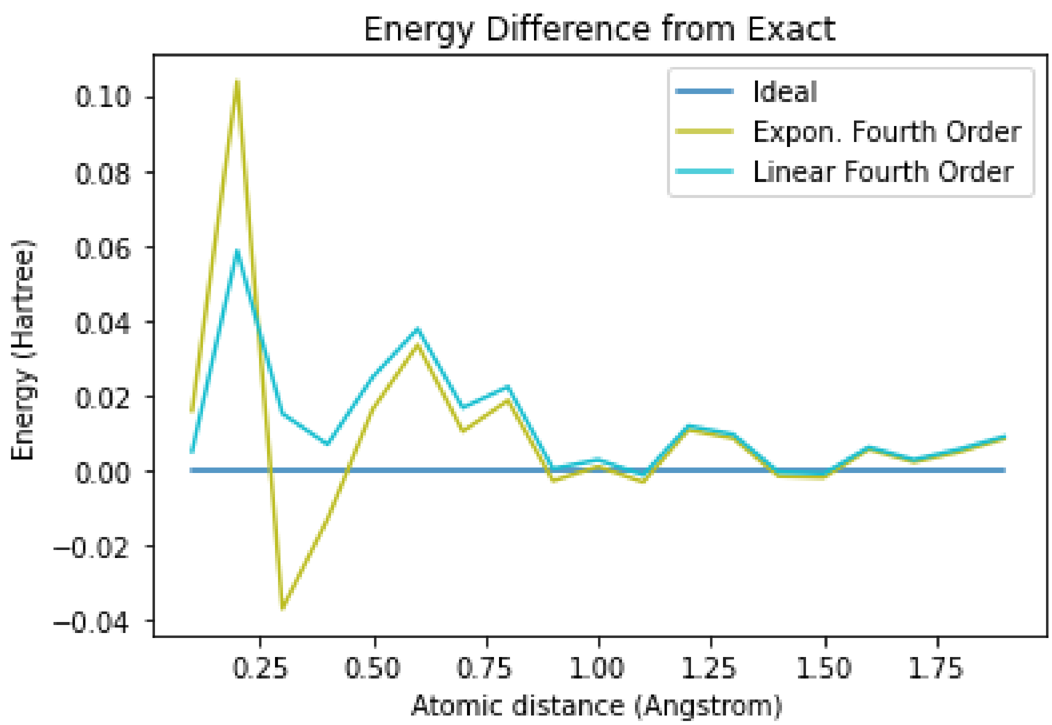
[41]:
```
plt.plot(distances, energy_difference[0], label="Ideal")
plt.plot(distances, ex_orders_diff[1], label="Expon. Second Order", color= 'tab:
 ↪olive')
plt.plot(distances, orders_diff[1], label="Linear Second Order", color= 'tab:
 ↪cyan')

plt.xlabel('Atomic distance (Angstrom)')
plt.ylabel('Energy (Hartree)')
plt.title('Energy Difference from Exact')
plt.legend()
plt.show()
```



[42]:
```
plt.plot(distances, energy_difference[0], label="Ideal")
plt.plot(distances, ex_orders_diff[2], label="Expon. Third Order", color= 'tab:
→olive')
plt.plot(distances, orders_diff[2], label="Linear Third Order", color= 'tab:
→cyan')

plt.xlabel('Atomic distance (Angstrom)')
plt.ylabel('Energy (Hartree)')
plt.title('Energy Difference from Exact')
plt.legend()
plt.show()
```



[43]:
```
plt.plot(distances, energy_difference[0], label="Ideal")
plt.plot(distances, ex_orders_diff[3], label="Expon. Fourth Order", color= 'tab:
 ↪olive')
plt.plot(distances, orders_diff[3], label="Linear Fourth Order", color= 'tab:
 ↪cyan')

plt.xlabel('Atomic distance (Angstrom)')
plt.ylabel('Energy (Hartree)')
plt.title('Energy Difference from Exact')
plt.legend()
plt.show()
```

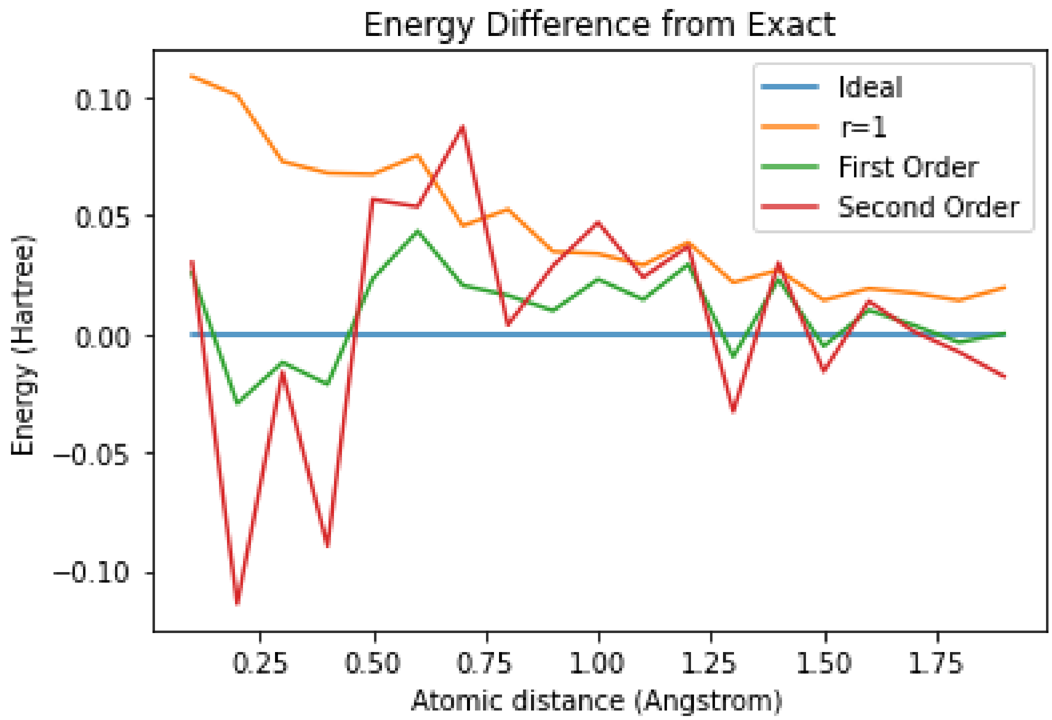


9 Extrapolating Using Equations

THIS IS NOT WORKING!!!!

[49]:
```
# extrapolating to 4 orders the entire thing through curve fitting
eq_orders = []
eq_orders_diff = []
#first Order
f_order = []
for i in range(len(vqe_ideal_energy)):
    answer = 2*(vqe_energies[0][i])-(vqe_energies[1][i])
    f_order.append(answer)
eq_orders.append(f_order)
#second order
s_order = []
for i in range(len(vqe_ideal_energy)):
    answer = (3*(vqe_energies[0][i]))-(3*(vqe_energies[1][i]))+vqe_energies[2][i]
    s_order.append(answer)
eq_orders.append(s_order)
#third order
t_order = []
for i in range(len(vqe_ideal_energy)):
```

```
    answer =␣
↪(4*(vqe_energies[0][i]))-(6*(vqe_energies[1][i]))+(4*vqe_energies[2][i])-vqe_energies[3][i]
    t_order.append(answer)
eq_orders.append(t_order)
#fourth order
fo_order = []
for i in range(len(vqe_ideal_energy)):
    answer =␣
↪(5*(vqe_energies[0][i]))-(10*(vqe_energies[1][i]))+(10*vqe_energies[2][i])-(5*vqe_energies[3]
↪(1*vqe_energies[4])                [i]
    fo_order.append(answer)
eq_orders.append(fo_order)
#differences from exact
for order in eq_orders:
    some_diff = []
    for k in range(len(vqe_ideal_energy)):
        some_diff = some_diff + [order[k] - exact_energies[k]]
    eq_orders_diff.append(some_diff)
#plotting energy differences
plt.plot(distances, energy_difference[0], label="Ideal")
plt.plot(distances, energy_difference[1], label="r=1")
plt.plot(distances, eq_orders_diff[0], label="First Order", color= 'tab:green')
plt.plot(distances, eq_orders_diff[1], label="Second Order", color= 'tab:red')
#plt.plot(distances, eq_orders_diff[2], label="Third Order", color = 'tab:
↪purple')
#plt.plot(distances, eq_orders_diff[3], label="Fourth Order", color = 'tab:pink')


plt.xlabel('Atomic distance (Angstrom)')
plt.ylabel('Energy (Hartree)')
plt.title('Energy Difference from Exact')
plt.legend()
plt.show()
```



Energy Difference from Exact
Ideal
r=1
First Order
Second Order
0.10
0.05
0.00
−0.05
−0.10
Energy (Hartree)
0.25
0.50
0.75
1.00
1.25
1.50
1.75
Atomic distance (Angstrom)


```
[ ]:
```