512Assignment1

September 20, 2019

Problem 1: We saw in class how Taylor series/roundoff errors fight against each other when deciding how big a step size to use when calculating numerical derivatives. If we allow ourselves to evaluate our function f at four points (x± and x ± 2),

a) What should our estimate of the first derivative at x be? Rather than doing a complicated fit, I suggest thinking about how to combine the derivative from x ± with the derivative from x ± 2 to cancel the next term in the Taylor series.

[1]:
```
from IPython.display import Latex
Latex(r"""From Taylor expansion:\begin{eqnarray}
f(x+\delta)= f(x) + \delta f'(x) + \frac{\delta^2}{2} f''(x) +␣
 ↪\frac{\delta^{3}}{3!} f'''(x) + \frac{\delta^{4}}{4!} f'''(x) +␣
 ↪\mathcal{O}(\delta^{5}) \\
f(x-\delta)= f(x) - \delta f'(x) + \frac{\delta^2}{2} f''(x) -␣
 ↪\frac{\delta^{3}}{3!} f'''(x) + \frac{\delta^{4}}{4!} f'''(x) -␣
 ↪\mathcal{O}(\delta^{5}) \\
f(x+\delta)-f(x-\delta)= 2\delta f'(x) + \frac{2\delta^{3}}{3!} f'''(x) +␣
 ↪\mathcal{O}(\delta^{5}) \\
f(x+\delta)-f(x-\delta)= 2\delta f'(x) + \frac{\delta^{3}}{3} f'''(x) +␣
 ↪\mathcal{O}(\delta^{5}) \\
\frac{f(x+\delta)-f(x-\delta)}{2\delta}= f'(x) + \frac{\delta^2}{6} f'''(x) +␣
 ↪\mathcal{O}(\delta^{4}) \\
\end{eqnarray}

Also from Taylor expansion but this time with 2
$\delta$:
\begin{eqnarray}
f(x+2\delta)-f(x-2\delta)= 4\delta f'(x) + \frac{8\delta^{3}}{3} f'''(x) +␣
 ↪\mathcal{O}(\delta^{5}) \\
\frac{f(x+2\delta)-f(x-2\delta)}{2\delta}= 2f'(x) + \frac{8\delta^2}{6}f'''(x)␣
 ↪+ \mathcal{O}(\delta^4) \\
\end{eqnarray}
Now, we combine the two:
\begin{eqnarray}
\frac{8(f(x+\delta)-f(x-\delta))-f(x+2\delta)+f(x-2\delta)}{2\delta}= 6f'(x) +␣
 ↪\mathcal{O}(\delta^{4})\\
\end{eqnarray}
Thus, the formula is:
```

```
\begin{eqnarray}f'(x)=\frac{8(f(x+\delta)-f(x-\delta))-f(x+2\delta)+f(x-2\delta)}{12\delta}+␣
↪\mathcal{O}(\delta^4)
\end{eqnarray}
""")
```

[1]: From Taylor expansion:

$$
\begin{aligned}
f(x+\delta) &= f(x)+\delta f'(x)+\frac{\delta^2}{2}f''(x)+\frac{\delta^3}{3!}f'''(x)+\frac{\delta^4}{4!}f'''(x)+\mathcal{O}(\delta^5) && (1)\\
f(x-\delta) &= f(x)-\delta f'(x)+\frac{\delta^2}{2}f''(x)-\frac{\delta^3}{3!}f'''(x)+\frac{\delta^4}{4!}f'''(x)-\mathcal{O}(\delta^5) && (2)\\
f(x+\delta)-f(x-\delta) &= 2\delta f'(x)+\frac{2\delta^3}{3!}f'''(x)+\mathcal{O}(\delta^5) && (3)\\
f(x+\delta)-f(x-\delta) &= 2\delta f'(x)+\frac{\delta^3}{3}f'''(x)+\mathcal{O}(\delta^5) && (4)\\
\frac{f(x+\delta)-f(x-\delta)}{2\delta} &= f'(x)+\frac{\delta^2}{6}f'''(x)+\mathcal{O}(\delta^4) && (5)\\
& && (6)
\end{aligned}
$$

Also from Taylor expansion but this time with 2 δ:

$$
\begin{aligned}
f(x+2\delta)-f(x-2\delta) &= 4\delta f'(x)+\frac{8\delta^3}{3}f'''(x)+\mathcal{O}(\delta^5) && (7)\\
\frac{f(x+2\delta)-f(x-2\delta)}{2\delta} &= 2f'(x)+\frac{8\delta^2}{6}f'''(x)+\mathcal{O}(\delta^4) && (8)\\
& && (9)
\end{aligned}
$$

Now, we combine the two:

$$
\begin{aligned}
\frac{8(f(x+\delta)-f(x-\delta))-f(x+2\delta)+f(x-2\delta)}{2\delta} &= 6f'(x)+\mathcal{O}(\delta^4) && (10)\\
& && (11)
\end{aligned}
$$

Thus, the formula is:

$$
f'(x)=\frac{8(f(x+\delta)-f(x-\delta))-f(x+2\delta)+f(x-2\delta)}{12\delta}+\mathcal{O}(\delta^4) \tag{12}
$$

[1]:
```python
#In code
import numpy as np
def firstderiv(x0,delta,fun):
    x=(x0-2*delta,x0-delta,x0+delta,x0+2*delta)
    y=fun(x)
    diff1= (y[2]-y[1])
    diff2= (y[3]-y[0])
    firstderiv= (8*diff1 -diff2)/(12*delta)
    return firstderiv

#Sanity Check
```

```python
fd=firstderiv(1,0.0000001,np.exp)
print("We find that d(exp(x))/dx evaluated at 1 is:",fd)
print("Which corresponds to our expectation of",np.exp(1))
print("The error is",abs(np.exp(1)-fd))
```

```
We find that d(exp(x))/dx evaluated at 1 is: 2.718281828887707
Which corresponds to our expectation of 2.718281828459045
The error is 4.286619947890813e-10
```

b) Now that you have your operator for the derivative, what should be in terms of the machine precision and various properties of the function?

[21]:

```python
from IPython.display import Latex
Latex(r"""To find the ideal delta, let's try to minimize our error:
\begin{eqnarray}diff=\frac{8(f(x+\delta)-f(x-\delta))-f(x+2\delta)+f(x-2\delta)}{12\delta}+␣
 ↪\mathcal{O}(\delta^4)\\
Error=|diff-f'(x)|\\
Error\approx|\frac{f^{(5)}\delta^4}{4}+\frac{\epsilon_mf(x)}{2\delta}|
\end{eqnarray}
Where the first term is the order of $\delta^4$ left from our expression of␣
 ↪diff, and $\epsilon_m$ is machine precision.
By minimizing this expression, we obtain:
\begin{eqnarray}
\frac{dError}{d\delta}=0 \\
0=f^{(5)}\delta^3-\frac{\epsilon_mf(x)}{\delta^2} \\
f^{(5)}\delta^3=\frac{\epsilon_mf(x)}{\delta^2} \\
\delta^5=\frac{\epsilon_mf(x)}{f^{(5)}} \\
\end{eqnarray}
So if we assume that $f(x)\approx f^{(5)}(x)$, then the ideal $\delta$ is␣
 ↪$\epsilon_m^{1/5}$, or $10^{-16/5}$.
""")
```

[21]:

To find the ideal delta, let's try to minimize our error:

$$diff=\frac{8(f(x+\delta)-f(x-\delta))-f(x+2\delta)+f(x-2\delta)}{12\delta}+\mathcal{O}(\delta^4) \tag{13}$$

$$Error=|diff-f'(x)| \tag{14}$$

$$Error\approx|\frac{f^{(5)}\delta^4}{4}+\frac{\epsilon_mf(x)}{2\delta}| \tag{15}$$

Where the first term is the order of δ^4 left from our expression of diff, and ϵ_m

is machine precision. By minimizing this expression, we obtain:

$$\frac{dError}{d\delta} = 0 \tag{16}$$

$$0 = f^{(5)}\delta^3 - \frac{\epsilon_m f(x)}{\delta^2} \tag{17}$$

$$f^{(5)}\delta^3 = \frac{\epsilon_m f(x)}{\delta^2} \tag{18}$$

$$\delta^5 = \frac{\epsilon_m f(x)}{f^{(5)}} \tag{19}$$

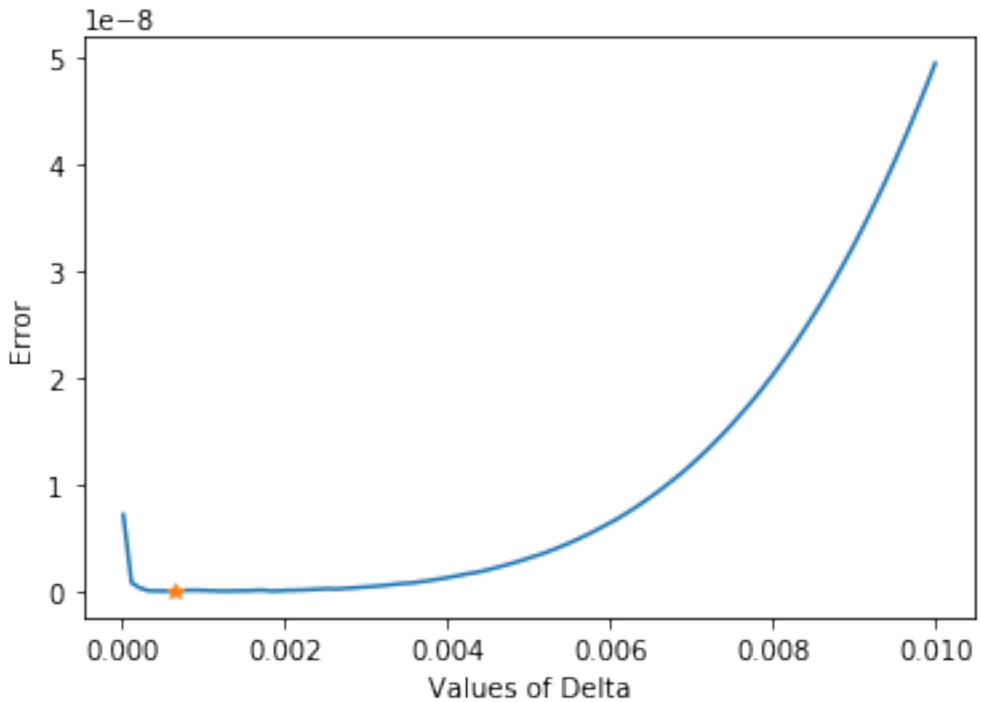
$$\tag{20}$$

So if we assume that $f(x) \approx f^{(5)}(x)$, then the ideal δ is $\epsilon_m^{1/5}$, or $10^{-16/5}$.

b) (continued) Show for f(x) = exp(x) and f(x) = exp(0.01x) that your estimate of the optimal is at least roughly correct.

[77]:

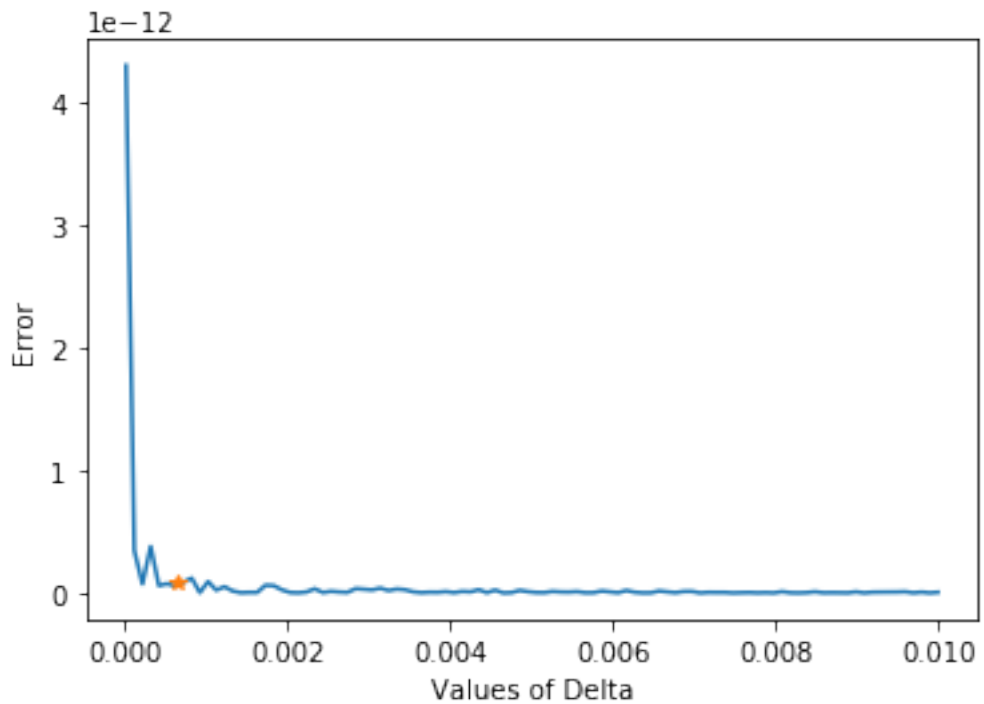
```
import numpy as np
from matplotlib import pyplot as plt
def firstderiv(x0,delta,fun):
    x=(x0-2*delta,x0-delta,x0+delta,x0+2*delta)
    y=fun(x)
    diff1= (y[2]-y[1])
    diff2= (y[3]-y[0])
    firstderiv= (8*diff1 -diff2)/(12*delta)
    return firstderiv

delta=np.linspace(10**(-5),10**(-2),100)
optimal_delta=(10**(-16/5))
error= abs(np.exp(5)-firstderiv(5,delta,np.exp))
optimal_error=abs(np.exp(5)-firstderiv(5,optimal_delta,np.exp))
plt.clf()
plt.plot(delta,error)
plt.plot((10**(-16/5)),optimal_error,"*")
plt.xlabel('Values of Delta')
plt.ylabel('Error')
plt.show()
print('Our optimal delta (orange point) roughly gives minimum error.')
```



Our optimal delta (orange point) roughly gives minimum error.

[79]:
```
import numpy as np
from matplotlib import pyplot as plt
def firstderiv(x0,delta,fun):
    x=(x0-2*delta,x0-delta,x0+delta,x0+2*delta)
    y=fun(x)
    diff1= (y[2]-y[1])
    diff2= (y[3]-y[0])
    firstderiv= (8*diff1 -diff2)/(12*delta)
    return firstderiv

def e001(x):
    y=np.exp(np.asarray(x)*0.01)
    return y

delta=np.linspace(10**(-5),10**(-2),100)
optimal_delta=(10**(-16/5))

exp001_A=0.01*np.exp(0.01) #analytical derivative
exp001_B=firstderiv(1,delta,e001) #using our algorithm and optimal delta
error2= abs(exp001_A-exp001_B)
optimal_error2=abs(0.01*np.exp(0.01)-firstderiv(1,optimal_delta,e001))
plt.clf()
```

```
plt.plot(delta,error2)
plt.plot(optimal_delta,optimal_error2,'*')
plt.xlabel('Values of Delta')
plt.ylabel('Error')
plt.show()
print('Our optimal delta (orange point) roughly gives minimum error.')
```

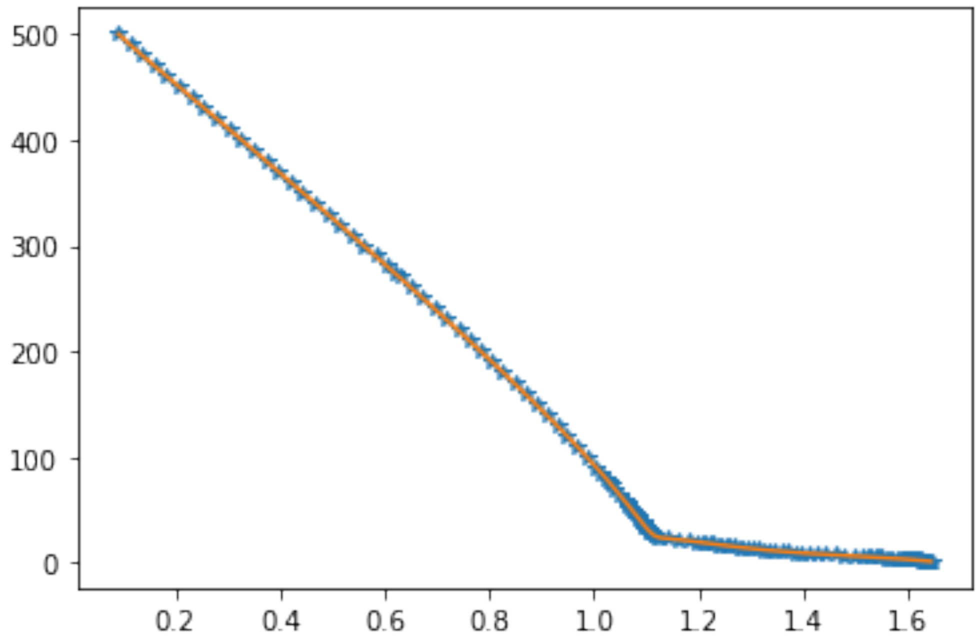


Our optimal delta (orange point) roughly gives minimum error.

Problem 2: Write a routine that will take an arbitrary voltage and interpolate to return a temperature.

[42]:
```
import numpy as np
from matplotlib import pyplot as plt
from scipy import interpolate


def temperature(V):
    data = np.loadtxt("/Users/jmlascar/lakeshore.txt")
    data = np.transpose(data)
    temperature, voltage = data[0], data[1]
    ind=np.argsort(voltage)
    temperature=temperature[ind]
    voltage=voltage[ind]
```

```
    spln=interpolate.splrep(voltage,temperature)
    yy=interpolate.splev(V,spln)
    return yy

def temperature_odd(V):
    data = np.loadtxt("/Users/jmlascar/lakeshore.txt")
    data = np.transpose(data)
    temperature, voltage = data[0], data[1]
    ind=np.argsort(voltage)
    temperature=temperature[ind]
    temperature=temperature[1::2]
    voltage=voltage[ind]
    voltage=voltage[1::2]
    spln=interpolate.splrep(voltage,temperature)
    yy=interpolate.splev(V,spln)
    return yy

#just to get a nice plot:
data = np.loadtxt("/Users/jmlascar/lakeshore.txt")
data = np.transpose(data)
temp, volt = data[0], data[1]
plt.clf()
plt.plot(volt, temp,"*")
plt.plot(volt,temperature(volt))
plt.show()

#estimate error



V=1.4
T=temperature(V)
error=abs(temperature_odd(V)-temperature(V))


if (V<9.0681e-02) or (V>1.64429):
    print("A voltage of",V,"V is outside the bounds of this interpolation.")
else:
    print("For a voltage of ",V,"V the temperature is",T,"K, and the error␣
 ↪is",error)
```



For a voltage of 1.4 V the temperature is 9.412486285451617 K, and the error is 9.26516856196713e-05

Problem 3) Write a recursive variable step size integrator like the one we wrote in class that does NOT call f(x) multiple times for the same x. For a few typical examples, how many function calls do you save vs. the lazy way we wrote it in class?

[59]:
```
import numpy as np

def myintegrate(fun,x1,x2,tracks=[[],[]],tol=1e-8):

    x = np.linspace(x1,x2,5) #get 5 points that are evenly spaced between a and␣
 ↪b
    y=[]
    neval=0

    if len(tracks[0])<1: #first time, when we haven't called the function at␣
 ↪all
        for i in x:
            y_i=fun(i)
            tracks[0].append(i)
            tracks[1].append(y_i)
            y.append(y_i)
            neval=neval+1
    else:
```

```
        for i in x:
            if i in tracks[0]: #function has already been called for that x
                index = tracks[0].index(i)
                y.append(tracks[1][index])
            else: #function has not been called for that x
                y_i=fun(i)
                tracks[0].append(i)
                tracks[1].append(y_i)
                y.append(y_i)
                neval=neval+1

    int1=(y[0]+4*y[2]+y[4])/6.0*(x2-x1)
    int2=(y[0]+4*y[1]+2*y[2]+4*y[3]+y[4])/12.0*(x2-x1)
    error=np.abs(int2-int1)

    if error<tol:
        return (16.0*int2-int1)/15.0,error,neval
    else:
        mid=0.5*(x1+x2)
        leftintegral,lefterror,leftneval=myintegrate(fun,x1,mid,tracks,tol/2.0)
        rightintegral,righterror,rightneval=myintegrate(fun,mid,x2,tracks,tol/2.
 ↪0)
        neval=neval+leftneval+rightneval
        integral=leftintegral+rightintegral
        error=lefterror+righterror
        return integral,error,neval

#######WAY WE DID IN CLASS FOR COMPARISON:#######

def simple_integrate(fun,a,b,tol=10e-8):
    x=np.linspace(a,b,5)
    #np.median(np.diff(x))
    y=fun(x)
    neval=len(x) #let's keep track of function evaluations
    f1=(y[0]+4*y[2]+y[4])/6.0*(b-a)
    f2=(y[0]+4*y[1]+2*y[2]+4*y[3]+y[4])/12.0*(b-a)
    myerr=np.abs(f2-f1)
    if (myerr<tol):
        #return (f2)/1.0,myerr,neval
        return (16.0*f2-f1)/15.0,myerr,neval
    else:
        mid=0.5*(b+a)
        f_left,err_left,neval_left=simple_integrate(fun,a,mid,tol/2.0)
        f_right,err_right,neval_right=simple_integrate(fun,mid,b,tol/2.0)
        neval=neval+neval_left+neval_right
        f=f_left+f_right
        err=err_left+err_right
```

```
        return f,err,neval

###############################
def exp2(x):
    y=np.exp(x**3)
    return y

def exp3(x):
    y=np.exp(-x)
    return y

intx=myintegrate(np.exp,0,2)
intclass=simple_integrate(np.exp,0,2)

intx2=myintegrate(exp2,0,2)
intclass2=simple_integrate(exp2,0,2)

print("Exp(x) integrated from 0 to 2: If we use our integral, we get", intx[2],␣
↪"function calls,",intclass[2]-intx[2],"less than with the one done in class.
↪")
print("Exp(x^3) integrated from 0 to 2:",intclass2[2]-intx2[2],"less function␣
↪calls.")
```

```
Exp(x) integrated from 0 to 2: If we use our integral, we get 257 function
calls, 58 less than with the one done in class.
Exp(x^3) integrated from 0 to 2: 4135 less function calls.
```

Problem 4

[74]:
```
from IPython.display import Latex
Latex(r"""For an infinitesimally thin shell of radius R and charge density␣
↪$\sigma$,
the field E in spherical coordinates only has a z component:
\begin{eqnarray}E=\frac{1}{4\pi\epsilon_0}\int \frac{\sigma R^2 sin\theta␣
↪d\theta d\phi (z-Rcos\theta)}{(R^2+z^2-2Rzcos\theta)^{3/2}} \\
\int d\phi = 2\pi \\
E =\frac{R^2\sigma}{2\epsilon_0}\int_0^{\pi} \frac{␣
↪(z-Rcos\theta)}{(R^2+z^2-2Rzcos\theta)^{3/2}}d\theta \\
u=cos\theta \\
du= -sin\theta d\theta \\
E =\frac{R^2\sigma}{2\epsilon_0}\int_{-1}^{1} \frac{ (z-Ru)}{(R^2+z^2-2Ru)^{3/
↪2}}du \\
\end{eqnarray}

""")
```

[74]:

For an infinitesimally thin shell of radius R and charge density σ, the field E in spherical coordinates only has a z component:

$$E = \frac{1}{4\pi\epsilon_0}\int \frac{\sigma R^2 sin\theta d\theta d\phi(z - Rcos\theta)}{(R^2 + z^2 - 2Rzcos\theta)^{3/2}} \tag{21}$$

$$\int d\phi = 2\pi \tag{22}$$

$$E = \frac{R^2\sigma}{2\epsilon_0}\int_0^{\pi} \frac{(z - Rcos\theta)}{(R^2 + z^2 - 2Rzcos\theta)^{3/2}}d\theta \tag{23}$$

$$u = cos\theta \tag{24}$$

$$du = -sin\theta d\theta \tag{25}$$

$$E = \frac{R^2\sigma}{2\epsilon_0}\int_{-1}^{1} \frac{(z - Ru)}{(R^2 + z^2 - 2Ru)^{3/2}}du \tag{26}$$

$$\tag{27}$$

[66]:
```
import numpy as np
from scipy import integrate
z=np.linspace(1,4,1)

R=2 #radius
sigma=3 #charge density
epsilon=8.85400e-12 #vacuum permittivity

def integral_mine(z,sigma,R=3,epsilon=8.85400e-12 ):
    #z: distance from center of the sphere at which the field is evaluated
    #theta: sheet charge density
    #R: radius of the shell
    #epsilon: permittivity of vacuum

    def integrand(u):
        y=(z-R*u)/((R**2+z**2-2*R*z*u)**(3/2))
        return y
    yy= (R**2*theta)/(2*epsilon)
    E= myintegrate(integrand, -1, 1)
    E= yy*E
    return E

def integral_quad(z,theta,R=3,epsilon=8.85400e-12 ):
    #z: distance from center of the sphere at which the field is evaluated
    #theta: sheet charge density
    #R: radius of the shell
    #epsilon: permittivity of vacuum
    def integrand(u):
        y=(z-R*u)/((R**2+z**2-2*R*z*u)**(3/2))
        return y
    yy= (R**2*theta)/(2*epsilon)
    E= scipy.integrate.quad(integrand, -1, 1)
```

```
    E= yy*E
    return E

E1= integral_mine(z,sigma)
E2= integral_quad(z,sigma)
print(E2)
print(E1)
```

```
      ␣
↪---------------------------------------------------------------------------

       RecursionError                            Traceback (most recent call␣
↪last)

       <ipython-input-66-434c993cc6ea> in <module>
        34     return E
        35
   ---> 36 E1= integral_mine(z,theta)
        37 E2= integral_quad(z,theta)
        38 print(E2)


       <ipython-input-66-434c993cc6ea> in integral_mine(z, theta, R, epsilon)
        17         return y
        18     yy= (R**2*theta)/(2*epsilon)
   ---> 19     E= myintegrate(integrand, -1, 1)
        20     E= yy*E
        21     return E


       <ipython-input-59-0350d4a222a2> in myintegrate(fun, x1, x2, tracks, tol)
        34     else:
        35         mid=0.5*(x1+x2)
   ---> 36         ␣
↪leftintegral,lefterror,leftneval=myintegrate(fun,x1,mid,tracks,tol/2.0)
        37         ␣
↪rightintegral,righterror,rightneval=myintegrate(fun,mid,x2,tracks,tol/2.0)
        38         neval=neval+leftneval+rightneval


       <ipython-input-59-0350d4a222a2> in myintegrate(fun, x1, x2, tracks, tol)
        35         mid=0.5*(x1+x2)
        36         ␣
↪leftintegral,lefterror,leftneval=myintegrate(fun,x1,mid,tracks,tol/2.0)
   ---> 37         ␣
↪rightintegral,righterror,rightneval=myintegrate(fun,mid,x2,tracks,tol/2.0)
```