

Vector Operations and Functions in Python

Assignment 2

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February 6, 2018
First created on January 31, 2018

Abstract

This report presents a study of different methods of creating a $\tan^{-1}(x)$ from its integral definition of $\int_0^x dx/(1+t^2)$ using scipy's quad function to integrate and other method is of numerical integration using trapezoidal rule, which can be used even for non-integrable functions to integrate it. And it also discusses the advantage of Vectorization of code compared to for loops and also on finding estimate errors when actual error is unknown i.e function is non-integrable by halving the stepsize till it reaches certain tolerance!.

1 Introduction

This report discusses 5 tasks in python to create $\tan^{-1}(x)$ from its integral definition in stepwise manner.

- Define $f(t) = 1/(1+t^2)$ as a function in Python that takes a vector argument
- Define a vector x that covers the region $0 \leq x \leq 5$ in steps of 0.1
- Plot $f(x)$ vs x using the Python function and the already defined vector x .
- Integrate $f(x)$ using quad function and compare it with $\arctan(X)$
- Use one of the Numerical methods i.e Trapezoidal rule to integrate $f(x)$ and to find estimate error and compare it with actual error

2 Python code

2.1 Code to create a tan inverse function from its integral definition

2.1.1 Integral definition of $\tan^{-1}(x)$ and plotting it

```
In [34]: #Importing libraries needed
from pylab import *
from scipy.integrate import quad
from math import pi
from tabulate import tabulate
#Function which takes vector x as argument used in calculation of tan inverse(x)

def f(x):
    return 1.0/(1+np.square(x))

#end of function

#Function to integrate f(x) from 0 to x[i](upper limit) using quad function for
#all elements in vector x, resulting answer is tan inverse(x[i]) using for loop
```

```

#method

def tan_inv(x):

    ans = np.zeros(len(x))          #initialising vector answer and error with zeros
    err = np.zeros(len(x))          #with length that of input vector x

    for i in range(len(x)):          #loop to calculate integral for all values of x
        ans[i],err[i] = quad(f,0,x[i])
    return ans,err

#end of function tan_inv

#declaring vector x
x = arange(0,5,0.1)
y = f(x)                            # y is another vecotr which stores vector returned by f(x)

#plotting f(x) vs x
fig1 = figure()
plot(x,y)
fig1.suptitle(r"Plot of  $1/(1+t^2)$ ", fontsize=20)
xlabel("x")
fig1.savefig('1.jpg')

#calculating tan inverse of all elements in x by arctan function
tan_inv_exact = np.arctan(x)

#plotting tan inverse vs x
fig2 = figure()
plot(x,tan_inv_exact)

#calculating tan_inverse through quad function and storing error associated
I_quad,err = tan_inv(x)

table = zip(tan_inv_exact,I_quad)
headers = ["arctan(x)", "quad_fn:integral"]
#tabulating arctan values vs quad function values
print tabulate(table,tablefmt="fancy_grid",headers=headers)

#plotting tan_inverse calculated using quad in same plot of arctan
plot(x,I_quad,'ro')
legend( (r"$tan^{-1}x$", "quad fn"))
fig2.suptitle(r"Plot of  $\tan^{-1}x$ ", fontsize=20)
xlabel("x")
ylabel(" $\int_0^x du/(1+u^2)$ ")
fig2.savefig('2.jpg')

#plotting error associated with quad function while calulating tan_inverse

fig3 = figure()
semilogy(x,abs((tan_inv_exact-I_quad)), 'r.')
fig3.suptitle(r"Error in  $\int_0^x dx/(1+t^2)$  ", fontsize=12)
xlabel("x")
ylabel("Error")
fig3.savefig('3.jpg')

show()

```

Figure 1: Graph of $f(x)$ vs x

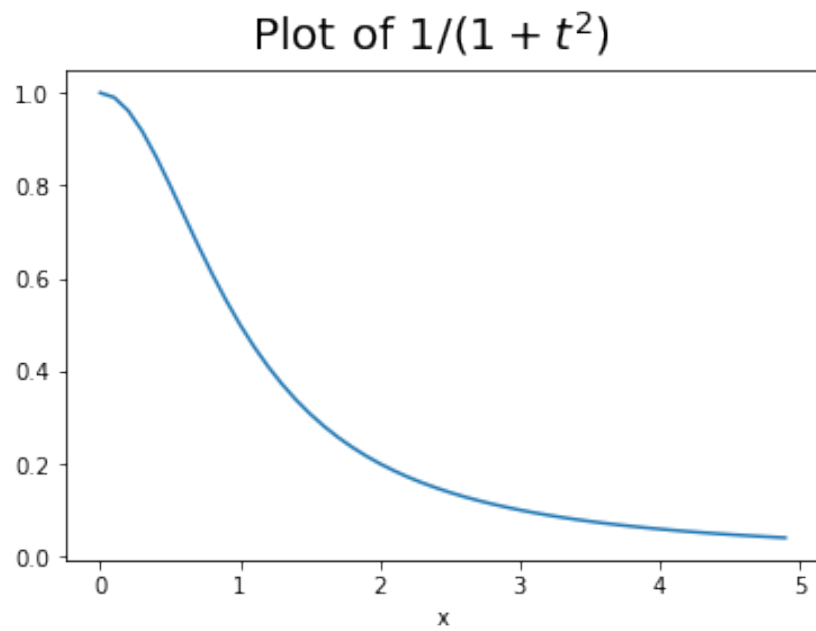
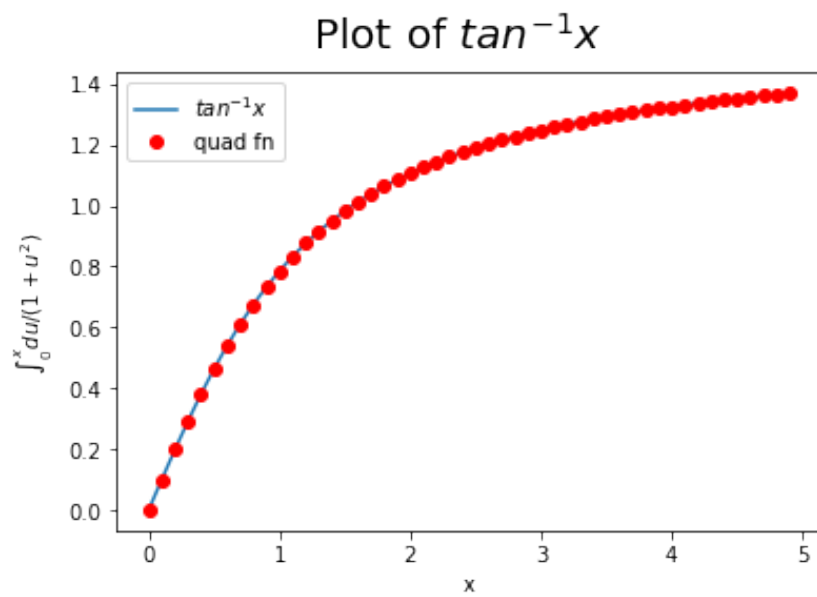


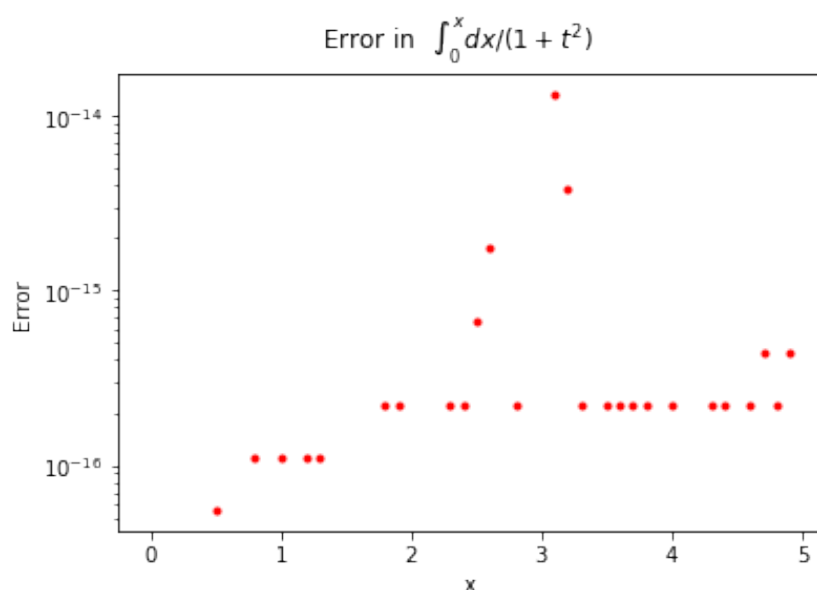
Figure 2: Comparison of $\tan^{-1}(x)$ and $\text{quad}(f(x))$ in same plot



Tabulating values of arctan(x) vs quad(f(x))

arctan(x)	quad : $\int_0^x dx/(1+t^2)$
0.00000	0.00000
0.09967	0.09967
0.19740	0.19740
0.29146	0.29146
0.38051	0.38051
0.46365	0.46365
0.54042	0.54042
0.61073	0.61073
0.67474	0.67474
0.73282	0.73282
0.78540	0.78540
0.83298	0.83298
0.87606	0.87606
0.91510	0.91510
0.95055	0.95055
0.98279	0.98279
1.01220	1.01220
1.03907	1.03907
1.06370	1.06370
1.08632	1.08632
1.10715	1.10715
1.12638	1.12638
1.14417	1.14417
1.16067	1.16067
1.17601	1.17601
1.19029	1.19029
1.20362	1.20362
1.21609	1.21609
1.22777	1.22777
1.23874	1.23874
1.24905	1.24905
1.25875	1.25875
1.26791	1.26791
1.27656	1.27656
1.28474	1.28474
1.29250	1.29250
1.29985	1.29985
1.30683	1.30683
1.31347	1.31347
1.31979	1.31979
1.32582	1.32582
1.33156	1.33156
1.33705	1.33705
1.34230	1.34230
1.34732	1.34732
1.35213	1.35213
1.35674	1.35674
1.36116	1.36116
1.36540	1.36540
1.36948	1.36948

Figure 3: Error associated with quad function compared to arctan(x)



2.2 Integration using Trapezoidal rule

2.2.1 Implementing with for loops without vectorization

```
In [38]: #Now we use numerical methods to calculate integral of f(x) using trapezoidal rule
#instead of quad function with for loops without vectorizing it
import time as t

#I is the vector which stores the integral values of f(x) using trapezoidal rule
I = []
h=0.1          #h is stepsize
x=arange(0,5,h) #x is input vector from 0 to 5 with stepsize 0.1

#Function which takes index of lower limit and upperlimit and stepsize as arguments
#and calculates using trapezoidal rule

def trapez(lower_index,i,h):
    Ii = h*((cumsumlike(i))-0.5*(f(x[lower_index])+f(x[i])))
    return Ii

#Its function to calculate cumulative sum till upper limit index i of input vector x
#this is implemented with for loop
def cumsumlike(i):
    temp=0
    for k in range(i):
        temp+=f(x[k])
    return temp

#noting down time it takes to run
t1 = t.time()
for k in range(len(x)):
    I.append(trapez(0,k,h))          #appending the values in vector
t2 = t.time()

print ("Time took without vectorization : %g" %(t2-t1))
#plotting Integral of x vs x
fig4 = figure()
plot(x,I,'r.')
fig4.suptitle(r"Trapezoid rule : $\int_0^x dx/(1+t^2)$ $",fontsize=12)
```

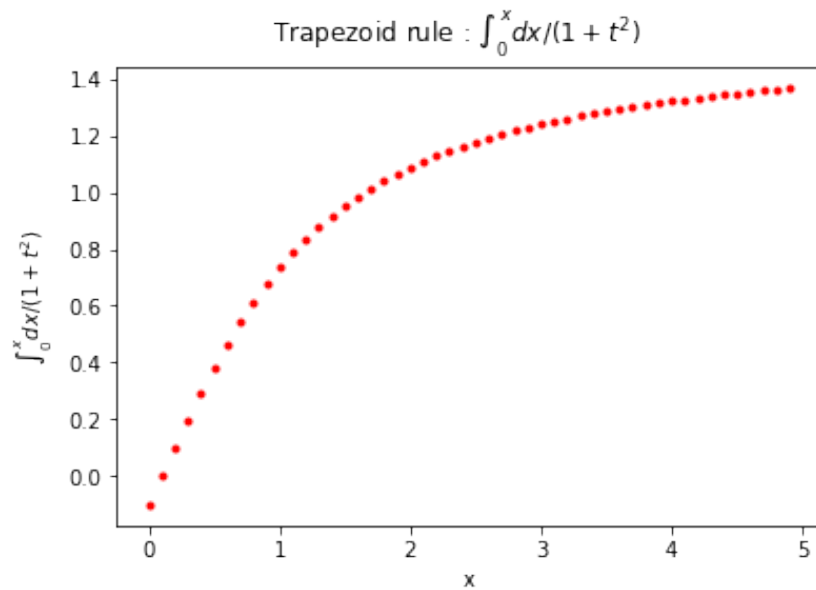
```

xlabel("x")
ylabel("$\int_0^x dx/(1+t^2)$")
fig4.savefig('4.jpg')
show()

```

Time took without vectorization : 0.005651

Figure 4: Plot of $\int_0^x dx/(1+t^2)$ using trapezoidal rule with loops



2.2.2 Trapezoidal rule using Vectorized Method

In [39]: *#Using Vectorized code and noting the time it takes to run*

```

t3 = t.time()
I_vect = h*(cumsum(f(x))-0.5*(f(x[0])+f(x)))          #vectorized code
t4 = t.time()

print ("Time took with vectorization : %g" %(t4-t3))
print ("Speed up factor while vectorizing code : %g" % ((t2-t1)/(t4-t3)))

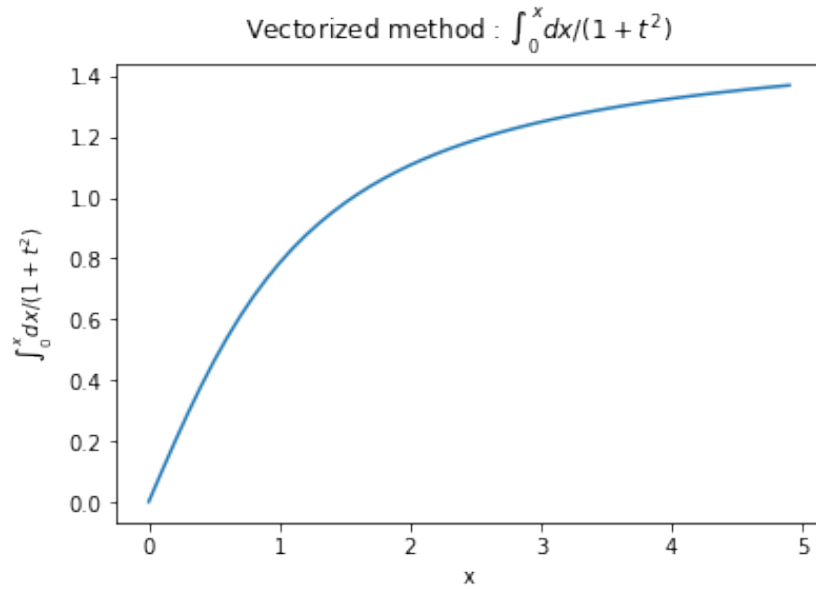
#plotting integral vs x using vectorized technique
fig5 = figure()
plot(x,I_vect)
fig5.suptitle(r"Vectorized method : $\int_0^x dx/(1+t^2)$",fontsize=12)
xlabel("x")
ylabel("$\int_0^x dx/(1+t^2)$")
fig5.savefig('5.jpg')
show()

```

Time took with vectorization : 0.000273943

Speed up factor while vectorizing code : 20.6284

Figure 5: Plot of $\int_0^x dx/(1+t^2)$ using trapezoidal rule after Vectorizing the code



2.2.3 Calculating Estimate error and Exact error associated with Trapezoidal rule by halving step-size

```
In [60]: #Estimating error by halving stepsize when greater the certain tolerance
          #initialising h vector

h = []
tol = 10**-8      #tolerance of 10^(-8)
est_err = []      #estimated error initialisation
act_err = []      #actual_error initialisation
i=0
h.append(0.5)

#while loop runs until est_err is less than tolerance

while(True):
    #temporary estimated_Error array,used to find max error among common points
    est_err_temp = []
    h.append(h[i]/2.0)          # halving h by 2
    x=arange(0,5,h[i])          # creating input with current stepsize
    x_next = arange(0,5,h[i+1]) #input with half of current stepsize

    #calculating Integrals with current h and h/2
    I_curr = h[i]*(cumsum(f(x))-0.5*(f(x[0])+f(x)))
    I_next = h[i+1]*(cumsum(f(x_next))-0.5*(f(x_next[0])+f(x_next)))

    #finding common elements
    x_com = np.intersect1d(x,x_next)

    #finding error between Integrals at common elements
    for k in range(len(x_com)):
        est_err_temp.append(I_next[2*k]-I_curr[k])

    #finding index of max error among common elements
    arg_max_err = argmax(abs(est_err_temp))

    #finding actual error and estimated error
    act_err.append(arctan(x_com[arg_max_err])-I_curr[arg_max_err])
```

```

est_err.append(est_err_temp[arg_max_err])

#incrementing i when est_error is greater than tolerance
if(est_err[i]>tol):
    i+=1
else:
    break;

#Tabulating h values vs est_error vs act_errors
table = zip(h,est_err,act_err)
headers = ["Stepsize h","Estimated Error","Actual Error"]
#tabulating arctan values vs quad function values
print tabulate(table,tablefmt="fancy_grid",headers=headers)

#printing the best value of h,it is last but index since its do-while loop
print"Best value of h is : %g" %(h[len(h)-2])

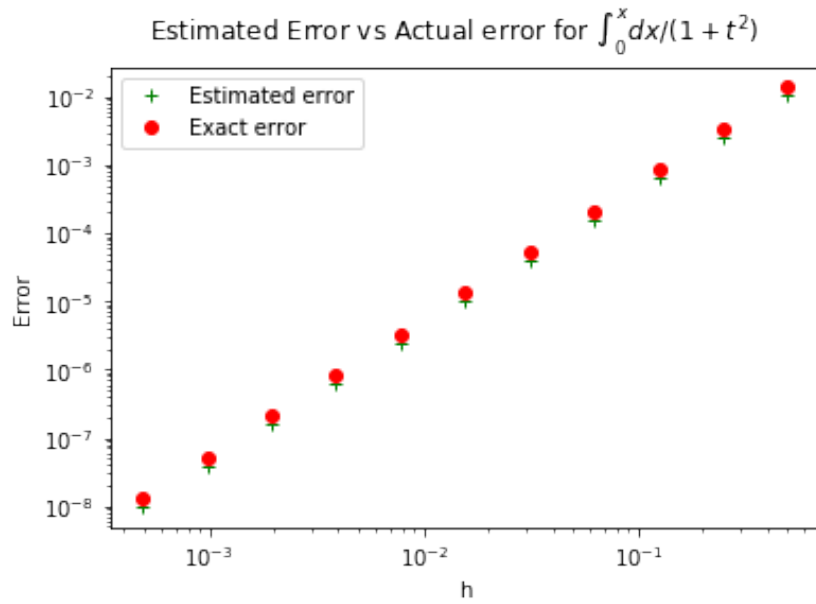
fig6 = figure()
loglog(h[:-1],est_err,'g+')
loglog(h[:-1],act_err,'ro')
legend(("Estimated error","Exact error"))
fig6.suptitle(r"Estimated Error vs Actual error for $\int_0^x dx/(1+t^2)$ $", fontsize=12)
xlabel("h")
ylabel("Error")
fig6.savefig('6.jpg')
show()

```

h	estimated error	exact error
0.5	0.0102941	0.0136476
0.25	0.00251891	0.00335349
0.125	0.000632009	0.000842472
0.0625	0.000158555	0.00021139
0.03125	3.96273e-05	5.28354e-05
0.015625	9.91109e-06	1.32147e-05
0.0078125	2.47773e-06	3.30364e-06
0.00390625	6.1943e-07	8.25906e-07
0.00195312	1.54857e-07	2.06476e-07
0.000976562	3.87144e-08	5.16191e-08
0.000488281	9.67859e-09	1.29048e-08

Best value of h is : 0.000488281

Figure 6: Comparison between Estimated Error and Exact Error in loglog plot



3 Results and Discussion

- So in this assignment we utilised the scientific python to do numerical computations like MATLAB and we saw that plotting and handling arrays and vectors were very simple.
- It also showcased that Vectorizing code improves the speed of the code by a great factor than using traditional for loops. And we also used scipy quad function to integrate a function and compared the error associated with it from actual value.
- And later we used Numerical methods to calculate integral of $f(x)$ by trapezoidal rule. This method is very useful since it can be used in case of Non-integral functions too!.
- And We also learnt how to find the Estimated Error from error between common points with different stepsizes which is very useful in case of non-integrable functions as exact values are not known.
- And we compared the Estimated Error and Exact Error and got to know that the estimated error (i.e., the maximum error on common points) is not equal to the actual error. This is an important thing to realise - numerical methods are always a little uncertain. Only in special cases do we know the exact error. With a function whose integral is not available, we have to depend on the estimated error to know when to stop.