भारतीय प्रौद्योगिकी संस्थान गुवाहाटी
INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

MA 322: Scientific Computing Lab

Lab 04

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Question 1.

In this question, we have to apply **Mid-point**, **Trapezoidal**, and **Simpson** methods to evaluate 3 integrals.

- Given $x_0 = a,\ x_1 = b$, the Midpoint rule is given by:
  $M(f) = (b-a)f\left(\frac{a+b}{2}\right)$
- Given $x_0 = a,\ x_1 = b$, the Trapezoid rule is given by:
  $T(f) = \frac{(b-a)}{2}(f(a) + f(b))$
- Given $x_0 = a,\ x_1 = \frac{(a+b)}{2},\ x_2 = b$, the Simpson rule is given by:
  $S(f) = \frac{(b-a)}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$

Using these 3 rules:

```
a. To integrate cos(x)/(cos(x)**2 + 1) from 0 to pi/2
   Evaluated value of integral using Midpoint rule is
   0.740480489693061
   Evaluated value of integral using Trapezoidal rule is
   0.392699081698724
   Evaluated value of integral using Simpson rule is
   0.624553353694949
   Exact value ≈ 0.623225

b. To integrate 1/(4*cos(x) + 5) from 0 to pi
   Evaluated value of integral using Midpoint rule is
   0.628318530717959
   Evaluated value of integral using Trapezoidal rule is
   1.74532925199433
   Evaluated value of integral using Simpson rule is
   1.00065543781008
   Exact value ≈ 1.047198

c. To integrate exp(-x**2) from 0 to 1
   Evaluated value of integral using Midpoint rule is
```

```
0.778800783071405
Evaluated value of integral using Trapezoidal rule is
0.683939720585721
Evaluated value of integral using Simpson rule is
0.747180428909510
Exact value ≈ 0.746824
```

Question 2.

Given the values of f:

x	1	1.25	1.50	1.75	2
f(x)	10	8	7	6	5

We will solve this question in 2 ways -

- Using composite rules
- Using normal rules (viz., endpoints 1 and 2 only)

Using composite rules:

In general,

Consider equally spaced nodes - $[x_0,\ x_1,\ x_2,\ \ldots,\ x_n]$,

- The composite Trapezoid rule is given as -
  $T(f) = h\left[\frac{f(x_0)}{2} + f(x_1) + \ldots + f(x_{n-1}) + \frac{f(x_n)}{2}\right]$
- The composite Simpson's rule is given as -
  $S(f) = \frac{h}{3}\left[f(x_0) + 2\sum_{j=2}^{n/2} f(x_{2j-2}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)\right]$

Using the above:

```
a. Evaluated value of integral using (composite) Trapezoidal rule
   is 7.125
b. Evaluated value of integral using (composite) Simpson rule is
   7.083333333333333
```

Using the normal rules (refer to question 1):

```
a. Evaluated value of integral using Trapezoidal (not composite)
   rule is 7.5
b. Evaluated value of integral using Simpson rule (not composite)
   is 7.166666666666667
```

Question 3.

Since in this case, we have been given an improper integral to approximate, we will first make a change of variables, viz, set $t = \frac{1}{1+x}$.

The integral $\int_0^\infty \frac{1}{x^2+9} dx$ now becomes, $\int_0^1 \frac{dt}{10t^2-2t+1}$.

Since n is given as 4, we get X = [0, 0.25, 0.50, 0.75, 1].

Applying the composite rules (refer to question 2.) -

```
a. Evaluated value of integral using composite Simpson rule is
   0.5205962059620596
b. Evaluated value of integral using composite Trapezoidal rule is
   0.5098915989159891
```

```
Note that the function when evaluated = , which is approximately
0.52359877559.
```

Question 4.

In this question, we will first evaluate the integral $\int_{-1}^1 \frac{1}{x+2} dx$

```
The actual value of the integral is 1.09861228866811
```

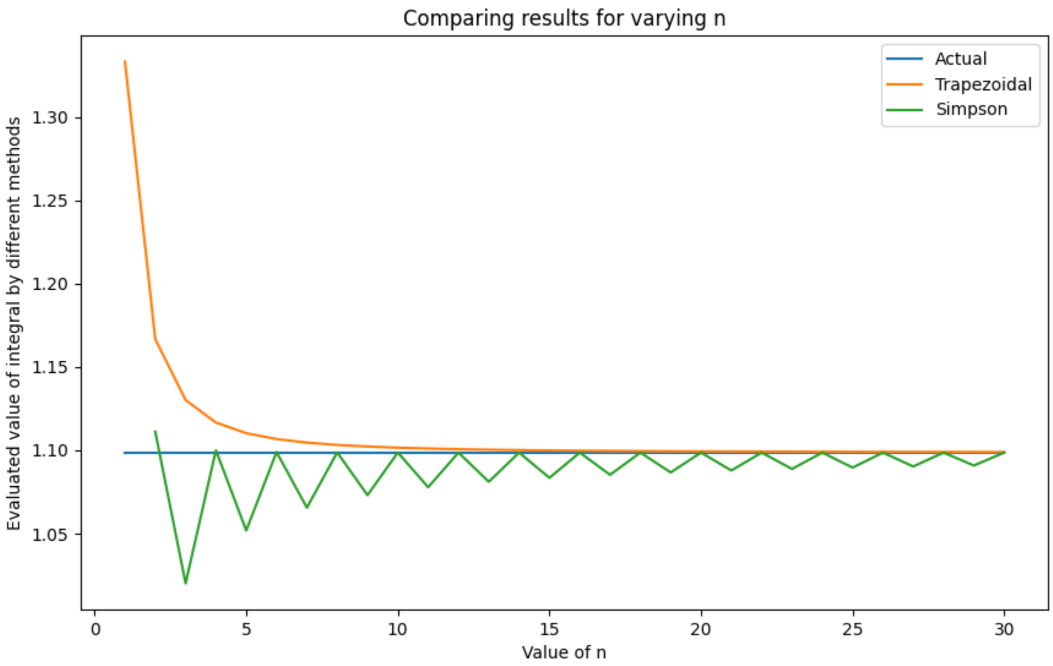
Now we perform the following analysis:

A. <u>Using composite Simpson and Trapezoidal rules and **varying n:**</u>
For this purpose, we take n from 1 to 30, and then in each case obtain the nodes X, and then apply the composite rules to obtain the estimated integral values. The values are tabulated below -

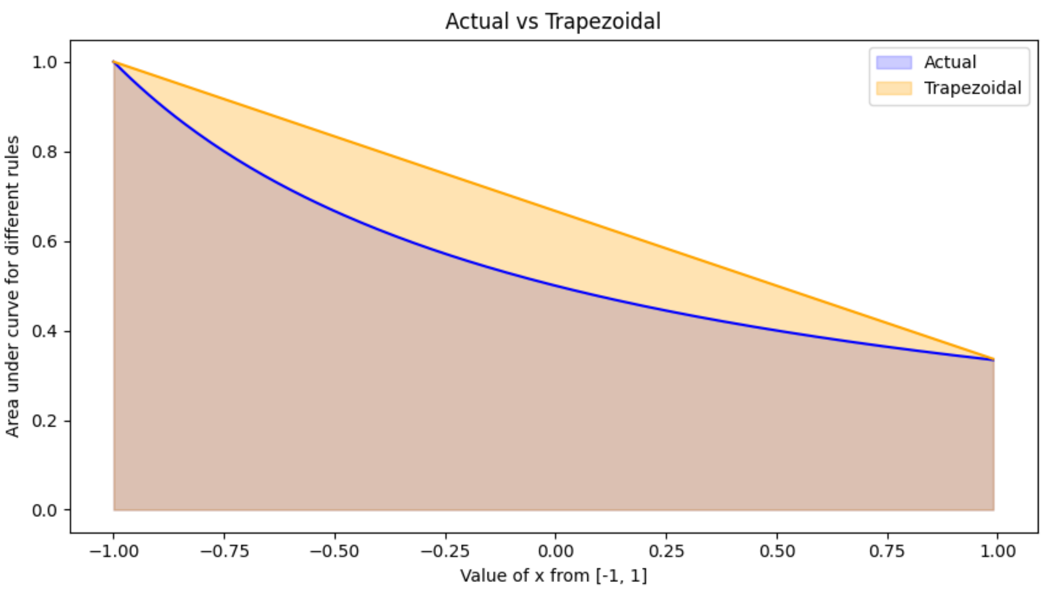
```
Terminal
imperial_lord@ab-notebook: ~/IITG/Semester 6/MA 322 (Scientific Computing Theory)/Labs/Lab 4
imperial_lord@ab-notebook:~/IITG/Semester 6/MA 322 (Scientific Computing Theory)/Labs/Lab 4$ python q4.py
Actual value of integral is 1.09861228866811

          Trapezoidal   Simpson
N-value
1.0          1.333333       NaN
2.0          1.166667  1.111111
3.0          1.130159  1.020106
4.0          1.116667  1.100000
5.0          1.110268  1.051867
6.0          1.106746  1.098942
7.0          1.104606  1.065548
8.0          1.103211  1.098725
9.0          1.102251  1.073081
10.0         1.101562  1.098661
11.0         1.101052  1.077833
12.0         1.100664  1.098636
13.0         1.100361  1.081098
14.0         1.100121  1.098625
15.0         1.099927  1.083479
16.0         1.099768  1.098620
17.0         1.099636  1.085290
18.0         1.099526  1.098617
19.0         1.099432  1.086715
20.0         1.099352  1.098616
21.0         1.099283  1.087865
22.0         1.099224  1.098614
23.0         1.099172  1.088812
24.0         1.099126  1.098614
25.0         1.099086  1.089606
26.0         1.099050  1.098613
27.0         1.099018  1.090281
28.0         1.098990  1.098613
29.0         1.098964  1.090862
30.0         1.098941  1.098613

imperial_lord@ab-notebook:~/IITG/Semester 6/MA 322 (Scientific Computing Theory)/Labs/Lab 4$
```

The plot, in this case, is obtained as below:

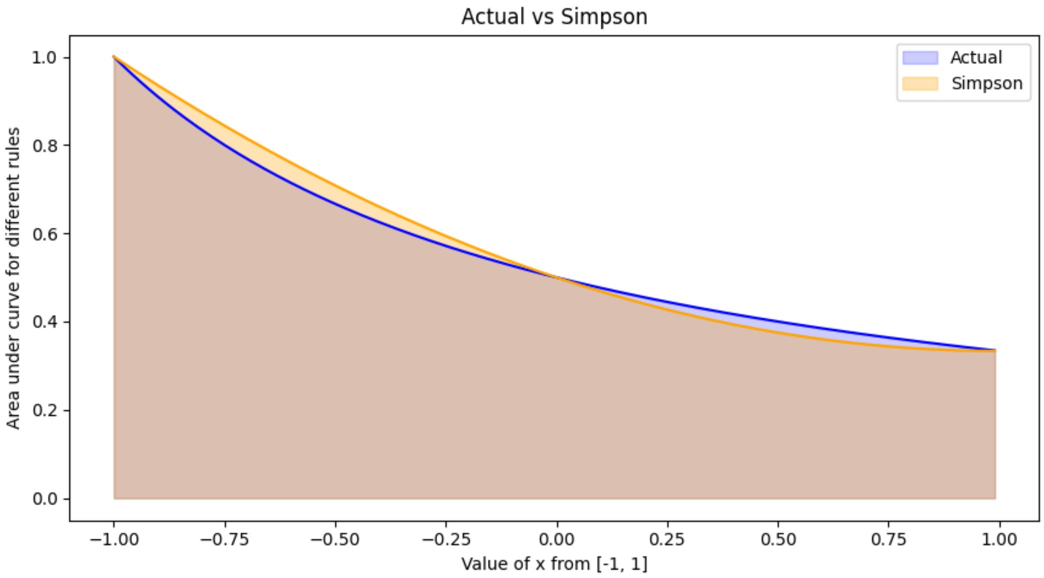
(PTO)



B. <u>Using Simpson and Trapezoidal rules **for the interval [-1,1]:**</u>
In this case, we will plot curves of 1/x+2 and also plot the parabola and trapezium obtained in the case of Simpson's and Trapezoidal rules respectively. We obtain the following graphs-



For the trapezium we join the points (-1,f(-1)) and (1,f(1)) and get -
$y = -\frac{1}{3}x + \frac{2}{3}$
For the parabola we join the points (-1,f(-1)), (0,f(0) and (1,f(1)) and get-
$y = \frac{1}{6}x^2 - \frac{1}{3}x + \frac{1}{2}$



Question 5.

For this question, we will use the error estimation for composite Trapezoidal, Simpson, and Midpoint rules.

- Composite Trapezoidal rule: $|E| \leq \frac{b-a}{12}h^2\left\|f^{(2)}\right\|_\infty$
- Composite Simpson rule: $|E| \leq \frac{b-a}{180}h^4\left\|f^{(4)}\right\|_\infty$
- Composite Midpoint rule: $|E| \leq \frac{b-a}{6}h^2\left\|f^{(2)}\right\|_\infty$

Using the error estimation formula in each case and setting the error $<10^{-5}$, we obtain the values of n and the corresponding value of h in each case. We also find the errors and observe that they are indeed $<10^{-5}$. The results are as follows:

```
The actual value of the integral is 0.405465108108164

For part a: (Trapezoidal Rule)
Constraints : h <= 0.0438178046004133 and n >= 46
Required tuple (n,h) with error < 0.00001 is (46,
0.0434782608695652l6)
The estimated value of integral is 0.4054705778040844
Error in this case is 5.46969592002400e-6

For part b: (Simpson Rule)
Constraints : h <= 0.44267276788012866 and n >= 6
Required tuple (n,h) with error < 0.00001 is (6, 0.3333333333333333)
The estimated value of integral is 0.4054663745840217
Error, in this case, is 1.26647585729778e-6

For part c: (Midpoint Rule)
Constraints : h <= 0.03098386676965934 and n >= 66
Required tuple (n,h) with error < 0.00001 is (66,
0.030303030303030304)
The estimated value of integral is 0.40546377960653796
Error, in this case, is 1.32850162642972e-6
```

Question 6.

For this question, we make use of composite trapezoidal rules, with a varying h, and keep decreasing h to h/2 unless -

$$\frac{\left|T(h)-T\left(\frac{h}{2}\right)\right|}{|T(h/2)|} < 10^{-6}$$

We start with h = b-a, and then store the previously computed values of f(x) in a map and re-use them whenever applicable. In each case, we have obtained the estimated value of integral, and the number of function evaluations needed. The results in each case are given below:

a.

```
For part a:

         h/2             T(h/2)  |T(h)-T(h/2)|/|T(h/2)|
0        1.5  0.917307692307692       0.509433962264151
1       0.75   1.09700436161776       0.163806704510337
2      0.375   1.13845856640156      0.0364125722333715
3     0.1875   1.14811803396732     0.00841330532225772
4    0.09375   1.15050088622580     0.00207114334895892
5   0.046875   1.15109475242811    0.000515914264279210
6   0.023438   1.15124310551227    0.000128863385544677
7   0.011719   1.15128018672115     3.22086745744655e-5
8   0.005859   1.15128945658244     8.05172082448184e-6
9    0.00293   1.15129177402021     2.01290222260620e-6
10  0.001465   1.15129235337794     5.03223809589083e-7

Estimated value of integral is 1.15129235337794
The total number of function evaluations f(x) is 2049
```

b.

```
For part b:

         h/2            T(h/2)  |T(h)-T(h/2)|/|T(h/2)|
0      0.475  5.89226190476190       0.692898272552783
1     0.2375  4.08369331873875       0.442875711974797
2    0.11875  3.35707584784789       0.216443566908585
3   0.059375  3.10177198119345      0.0823090376089534
4   0.029687  3.02413350261602      0.0256729666564883
5   0.014844  3.00299624330640     0.00703872319412089
6   0.007422  2.99755981998456     0.00181361629068801
7   0.003711  2.99618990900855    0.000457217672316779
8   0.001855  2.99584672967332    0.000114551699799879
9   0.000928  2.99576089054454     2.86535314135060e-5
10  0.000464  2.99573942798678     7.16436067594955e-6
11  0.000232  2.99573406217376     1.79115131995161e-6
12  0.000116  2.99573272070966     4.47791651650761e-7

Estimated value of integral is 2.99573272070966
The total number of function evaluations f(x) is 8193
```

c. (All 3 values of m = 0.5, 0.8, 0.95)

```
For part c.1 with m = 0.5:

        h/2            T(h/2)  |T(h)-T(h/2)|/|T(h/2)|
0  0.785398  1.85495913108563     0.0221890424223644
1  0.392699  1.85407522776731   0.000476735412394760
2   0.19635  1.85407467730167    2.96895075375513e-7

Estimated value of integral is 1.85407467730167
The total number of function evaluations f(x) is 9


For part c.2 with m = 0.8:

        h/2            T(h/2)  |T(h)-T(h/2)|/|T(h/2)|
0  0.785398  2.28474559207222      0.112422256104431
1  0.392699  2.25762152697275     0.0120144429770034
2   0.19635  2.25720546146261   0.000184327708417783
3  0.098175  2.25720532682087    5.96497509281531e-8

Estimated value of integral is 2.25720532682087
The total number of function evaluations f(x) is 17


For part c.3 with m = 0.95:

        h/2            T(h/2)  |T(h)-T(h/2)|/|T(h/2)|
0  0.785398  3.23285521032154      0.329414789501306
1  0.392699  2.94266734632302     0.0986138866022765
2   0.19635  2.90897327685914     0.0115828047414244
3  0.098175  2.90833756138449   0.000218583799588455
4  0.049087  2.90833724844466    1.07600942541519e-7

Estimated value of integral is 2.90833724844466
The total number of function evaluations f(x) is 33
```

Question 7.

a. This question has been solved mathematically as below:

Question 7(a).

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To derive an estimate of the error

$$E(f) = \left| \int_a^b f(x)dx - T(h) \right|$$

We know, that the error associated with trapezoidal rule is :-

$$E_{1,h}(f) = I(f) - T_n(f) = \frac{-h^2}{12}(b-a)\|f^2(\theta)\|_\infty$$

In the given question,

$$\hat{f}(x) = f(x) + \delta(x).$$

$$\Rightarrow E'_{1,h}(f) = I(f) - T_n(\hat{f})$$

$$= \left(I(f) - T_n(f)\right) - \frac{h}{2}\sum_{i=0}^{n-1}\left(\delta(x_i) + \delta(x_{i+1})\right)$$

$$= E_{1,h}(f) - \frac{h}{2}\sum_{i=0}^{n-1}\left(\delta(x_i) + \delta(x_{i+1})\right)$$

$$\Rightarrow E'_{1,h}(f) = \frac{-h^2}{12}(b-a)\|f''(\theta)\|_\infty - \frac{h}{2}\sum_{i=0}^{n-1}\left(\delta(x_i) + \delta(x_{i+1})\right)$$

$$\Rightarrow \boxed{\left|E'_{1,h}(f)\right| \leq \frac{h^2}{12}(b-a)\|f''(\theta)\|_\infty + (b-a)\delta}$$

(since, $|\delta(x_i)| \leq \delta \; \forall \; x_i$)

b. If we are given δ the only variable term will be h, and a smaller h would mean a smaller error. Thus, h should be reasonably small.

```
Using inexact function evaluations
Approximate value of integral for h=0.0002 is 0.25492149684495113
Error in the process: 0.004970556825512118
```

Using the function $f^{\Lambda}(x) = x^3 + 0.01 * rand$, we plot the error in estimation versus n and obtain the following graph:

Now, we see that for large values of n, the error becomes almost constant and is converging to a certain limit. And since n and h are inversely proportional, this implies that the step size should be small in value when δ is given.