PHY453: Computational Physics | Assignment 1

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Question A

I have computed the integral of

$$\left(\int_0^1 \frac{4\mathrm{dx}}{1+x^2}\right)$$

using the composite trapezoidal method. The source-code and compiled files for this exercise are labeled as `20181044_A_{x}_sourcecode.f90` and `20181044_A_{x}_compiled.x` respectively. Here '{x}' refers to the sub-question number.

The source-code can be compiled and checked by running:

```
>>> gfortran -o 20181044_A_{x}_compiled.x 20181044_A_{x}_sourcecode.f90
>>> ./20181044_A_{x}_compiled.x
```

A.3 Plot of Log-Absolute Error

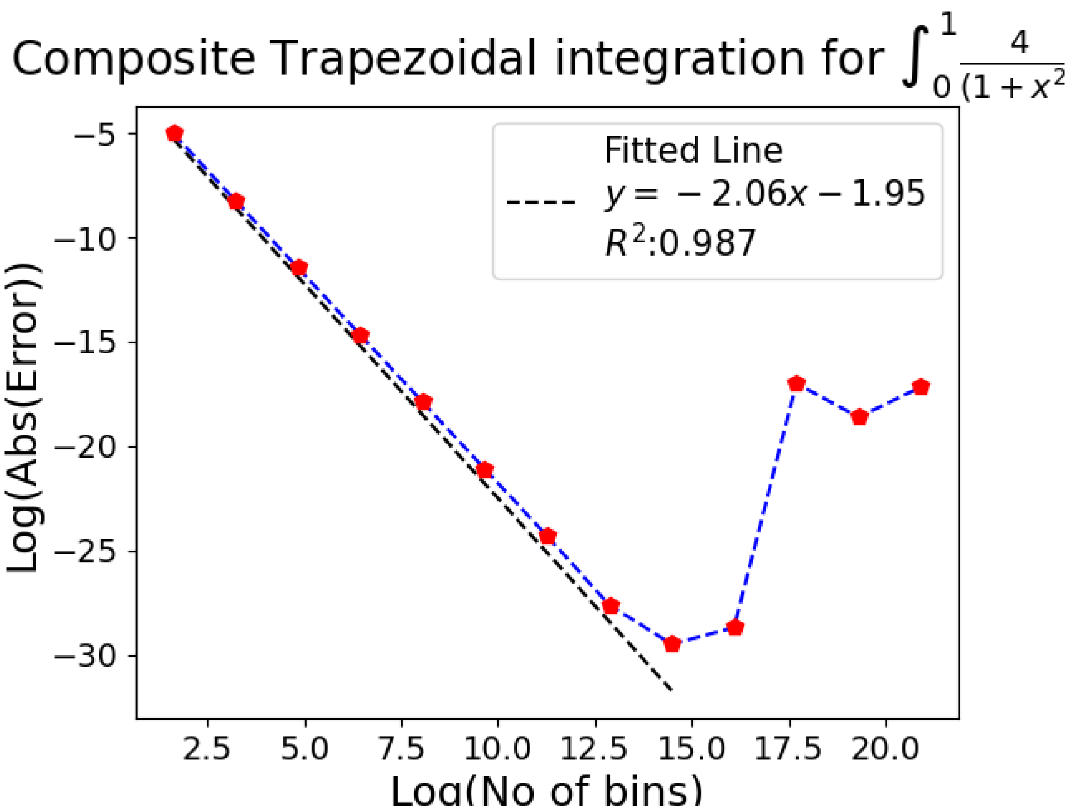

Figure 1: Plot of Logarithmic Absolute Error from `A_3_sourcecode.f90`

Observation:

- We notice the log-absolute error is always negative and linearly decreses in the log-log plot upto a certain number of bins. The negativity of the logarithmetic error signifies that the error is always lesser than 1.
- We can fit a linear plot upto a certain number of bins (here it is till $n = 5^8$). A linear fit in this regime has an R^2 of 0.987 which implies that the linear model explains the behaviour and varaince in data with high accuacy. The linear behaviour can be explained by the variation of LogN vs the Error value (Figure 2). After 5^9 bins, the error increases quadratically and this might be due to the behaviour of the function within very small bins. This can be checked and confirmed with higher floating values.

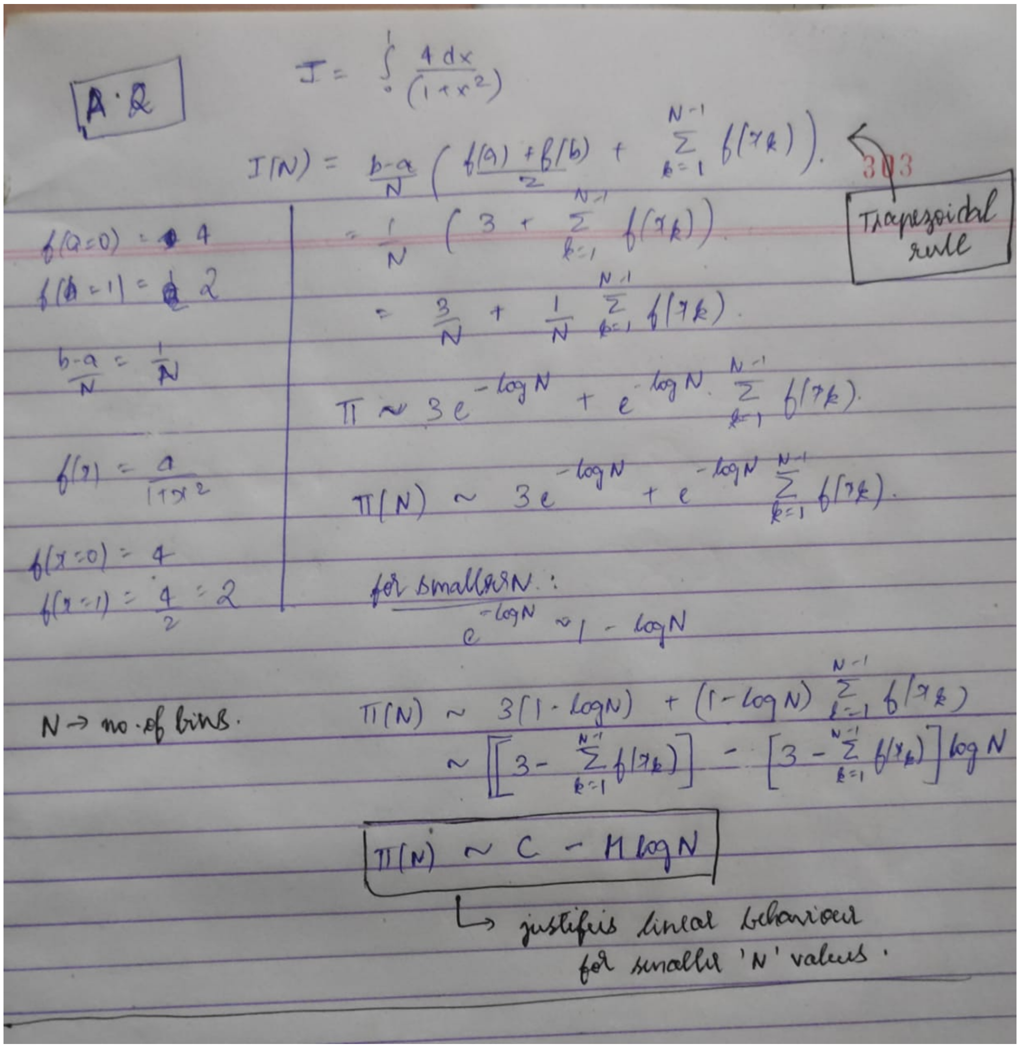

Figure 2: Explanation for Linear behaviur of error

Question B

The source-code for this question is at `20181044_B_sourcecode.f90`. The value of the integral comes out to be equal to 2.0 analytically. Using double-precision, we get a similar answer using the trapezoidal-method, only differing in higher decimal places. This confirms that the trapezoidal method works acurately.

Question C

The analytical value of the Gaussian integral with $\mu = 0$ and $\sigma = 1$ over the real axis is 1.0. However, with the given limits the integral converges to 1.0 with higher bin sizes. Furthermore, accuracy of the integral is higher with the larger limits ie (-5,5).

The outut of `./20181044_C_complied.x` is :

```
Welcome to this program.  This program does integration on
I= Int_a^b Gaus(0,1) using trapezoidal rule with n= 1000 bins
The integrated value using trapezoidal rule in (-3,3) is:  0.99730012416375569
The integrated value using trapezoidal rule in (-5,5) is:  0.99999942657296670
```

Question D

I have used the following definition for the error function:

$$\text{Erf(x)} = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du$$

We perform composite trapezoidal integration on e^{-u^2} using 10000 bins between x $\in (-3, 3)$ and a step size of 0.005 in double-precision. The code for this exercise is available at `20181044_D_sourcecode.f90`.

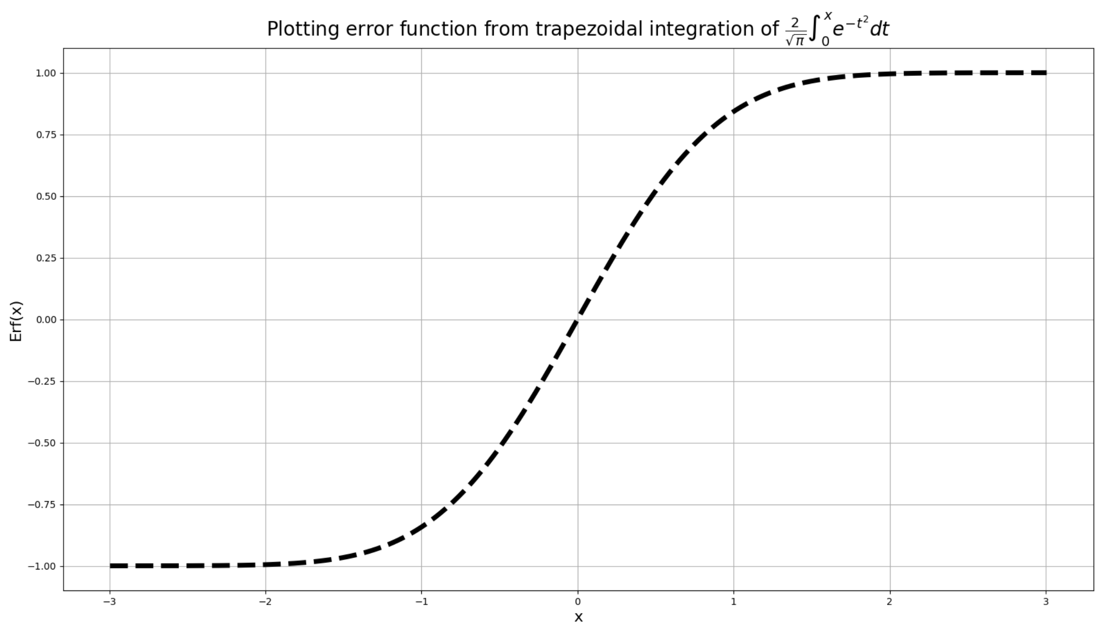

Figure 3: Plot of Error Function from `D_sourcecode.f90`