HW3

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1 What

The overall goal of this homework was to implement and experiment with different ways of numerically computing integrals. In this homework we will experiment with two different ways of computing approximate values of Integral: Trapezoid Rule and Gauss Quadrature.

2 How

Objective: After doing this homework we would have written a Python program from scratch to carry out numerical integration and gained some knowledge of the accuracy of some different methods for numerical integration (quadrature).

There are four code files: *trapezoidal.py*, *gauss.py*, *lglnodes.py*, and *drive.py*. Where, *trapezoid.py* implements a general Trapezoidal Rule, *gauss.py* implements a general Gauss quadrature, and then *drive* automates the process of running Trapezoid Rule and Gauss Quadrature and makes plots of n vs error.

$$I = \int_{-1}^{1} e^{cos(kx)} dx$$

A Python program uses Trapeqoidal rule and Gauss Quadrature to approximate the above integral for both $k = \pi$ and $k = \pi^2$ and for $n = 2, 3, ..., N$, where N is chosen so that the absolute error estimate $(\delta_{abs})_{n+1} = |I_{n+1} I_n|$ is smaller than 1010. The N is found experimentally roughly when the error estimate falls below 1010.

We will consider the integral of the function: $f(x) = e^{cos(kx)}$, with $k = \pi$ or $k = \pi^2$

2.1 Trapezoid Rule

The trapezoid rule belongs to the class of Newton-Cotes quadrature rules, which approximate integrals using equidistant grids. The rule uses a set of equidistant grid points.

$$I = \int_{-1}^{1} e^{cos(kx)} dx$$

A Python program that uses the trapezoid rule to approximate the above integral for both $k = \pi$ and $k = \pi^2$ and for $n = 2, 3, ..., N$, where N is chosen so that the absolute error estimate $(\delta_{abs})_{n+1} = |I_{n+1} I_n|$ is smaller than 1010. The N is found experimentally roughly when the error estimate falls below 1010.

We will consider the integral of the function: $f(x) = e^{cos(kx)}$, with $k = \pi$ or $k = \pi^2$

1. The value of N is determined experimentally by calculating error for different trials of grid points.

2. The error was plotted against the number of grid points on a log-log plot.

2.2 Gauss Quadrature

In NewtonCotes quadrature rules, it is assumed that the value of the integrand is known at equally spaced points. If it is possible to change the points at which the integrand is evaluated, other methods such as Gauss quadrature and ClenshawCurtis quadrature are often more suitable.

In Gauss quadrature, the location of the grid-points xi (usually referred to as quadrature nodes) and the quadrature weights ω_i are chosen so that the order of the approximation to the weighted integral is maximized, where the weight function $\omega(x)$ is assumed to be positive and integrable (in this homework $\omega(x) = 1$).

The error against n using a logarithmic scale for both axes was plotted (in the same figure).

For Gauss quadrature the error is expected to decrease as $\epsilon(n) = C^{\alpha n}$

The values of C and α we tried were: 1.5, 2, and 2.5 for C and α

2.3 Why: Trapezoidal Rule

1. The trapezoidal rule results were printed for function 1 (with $k = \pi$) and function 2 (with $k = \pi^2$)

2. Firstly, as seen in Figure 1, the use of trapezoidal rule to evaluate the integral of function 1 required 10 evaluations with n=2,3,..,11 trapezoids to satisfy the error tolerance 1e-10. The convergence is seen to be exponential which can be explained by the function being periodic.

3. Secondly, as seen in Figure 2, the use of trapezoidal rule to evaluate the integral of function 2 required 998 evaluations with n=2,3,..,999 trapezoids to satisfy the error tolerance 1e-10. The order of convergence was between n^{-2} and n^{-3}

2.4 Why: Gauss Quadrature

1. The Gauss plots shown display the error in approximation using Gauss quadrature as a function of the number of weights and nodes, n for the first and second functions of x, respectively.

2. Alongside the Gauss quadrature approximation error function, we have provided plots of n^{-2}, $n^(-4)$ and $n^(-n)$ for reference. We can observe that the behavior of the Gauss quadrature approximation error function is most similar to $n^(-n)$ and is approaching 0 significantly faster than $n^(-2)$ and $n^(-4)$. This tells us that Gauss quadrature is converging to the exact integral at an exponential order. This general convergence holds for both functions of x.

3. For the first function of x, we can observe a slight initial increase in error before converging to an error of approximately $10^(-16)$ at n approximately $10^(1.5)$.

4. For the second function of x, we can observe a slightly more noticeable initial increase in error with some fluctuations before converging to an error of approximately $10^(-16)$ at n approximately $10^(2)$.

5. The Gauss Quadrature rule results were printed for function 1 (with $k = \pi$) and function 2 (with $k = \pi^2$)

6. Firstly, as seen in Figure 3, the use of Gauss Quadrature rule to evaluate the integral of function 1 required 18 evaluations with n=2,3,..,19 weights/nodes to satisfy the error tolerance 1e-10.

7. Secondly, as seen in Figure 4, the use of Gauss quadrature rule to evaluate the integral of function 2 required 52 evaluations with n=2,3,..,53 weights/nodes to satisfy the error tolerance 1e-10. The order of convergence was between n^{-2} and n^{-3}

8. Lastly, for Gauss quadrature the error is expected to decrease as $\epsilon(n) = C^{\alpha n}$. As shown in Figures 6 and **??** the values of C and α we tried were: 1.5, 2, and 2.5 for C and α, for functions 1 and 2. For function 1, the error approximately follows $\epsilon(n) = 2^{2n}$. For function 2, the error approximately follows $\epsilon(n) = 1.5^{1.5n}$.

3 Cost Comparison

1. The The trapezoidal rule is exponentially (geometrically) convergent for periodic functions. Evaluating I for $k = \pi$ is a case in point of Euler-Maclaurin formula which can be used to approximate integrals by finite sums. Therefore, as seen in 1, the error converges exponentially rather than quadratically. The errors for the integrals over periodic functions roughly cancel after one cycle.

2. To compare accuracy between the Trapezoidal Rule and Gauss Quadrature, we can evaluate how many evaluations are necessary to get within tolerance 10^-5 and 10^{-10} and compare the number of evaluations needed for each method with each tolerance. We can do this for both functions of x and observe how these functions affect the number of evaluations needed. The output from this evaluation is below.

    - The trapezoidal rule on function 1 required 10 evaluations with n=2,3,..,11 trapezoids to satisfy the error tolerance 1e-10.
    - Gauss quadrature on function 1 required 18 evaluations with n=2,3,..,19 weights/nodes to satisfy the error tolerance 1e-10.
    - The trapezoidal rule on function 2 required 998 evaluations with n=2,3,..,999 trapezoids to satisfy the error tolerance 1e-10.
    - Gauss quadrature on function 2 required 52 evaluations with n=2,3,..,53 weights/nodes to satisfy the error tolerance 1e-10.

3. Average Gauss Evaluations: (19 + 53) / 2 = 45.5 Average Trapezoidal Rule Evaluations: (11 + 909) / 2 = 505

4. In a general setting we can conclude that Gauss may be more efficient as it averages to consistently better behavior, however, if we have periodic functions trapezoid rule can perform very well as seen with function 1 ($k = \pi$).

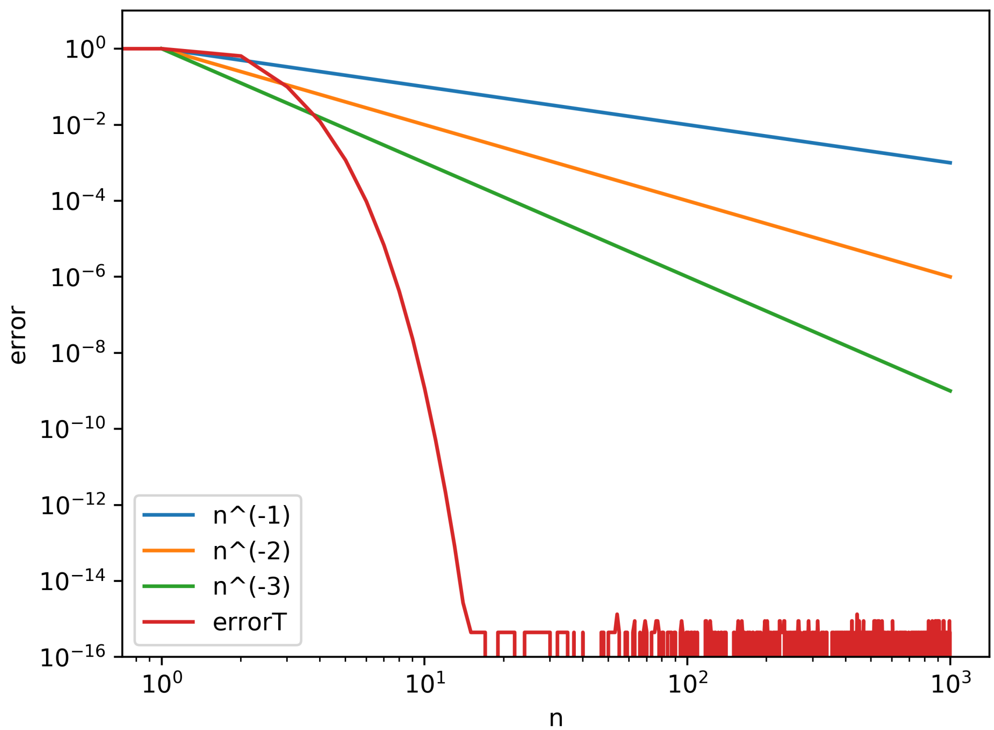

Figure 1: This figure shows the log-log plot of convergence of error for trapezoidal rule used for evaluating I with $k = \pi$, showing comparison to quadratic and exponential convergence

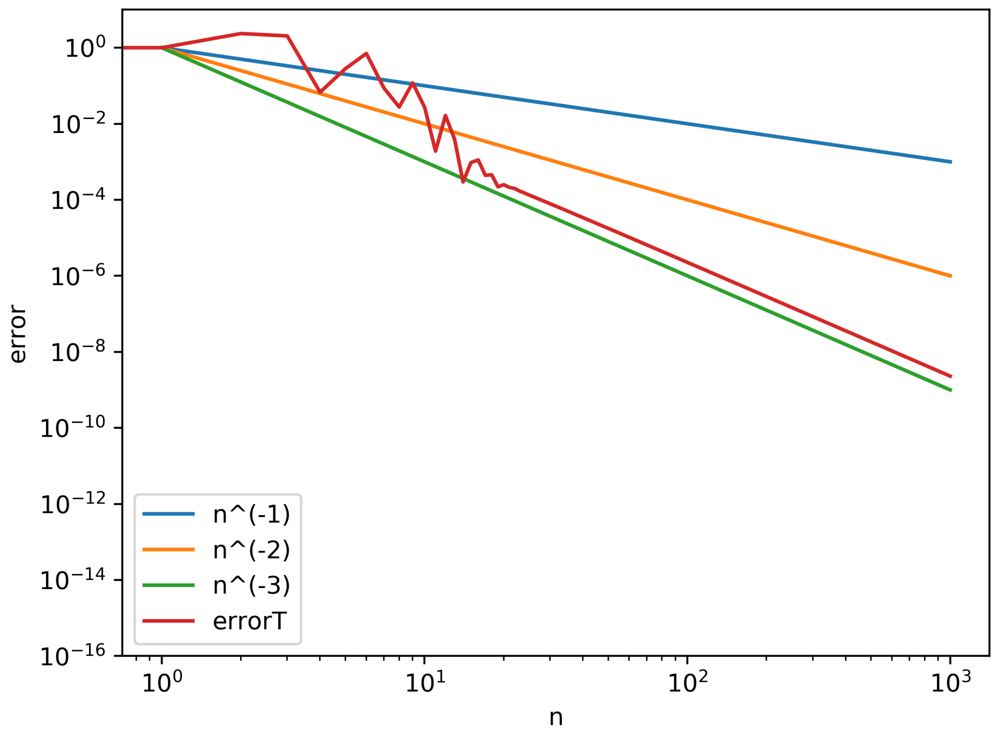

Figure 2: This figure shows the log-log plot of convergence of error for trapezoidal rule used for evaluating I with $k = \pi^2$, showing comparison to quadratic and exponential convergence

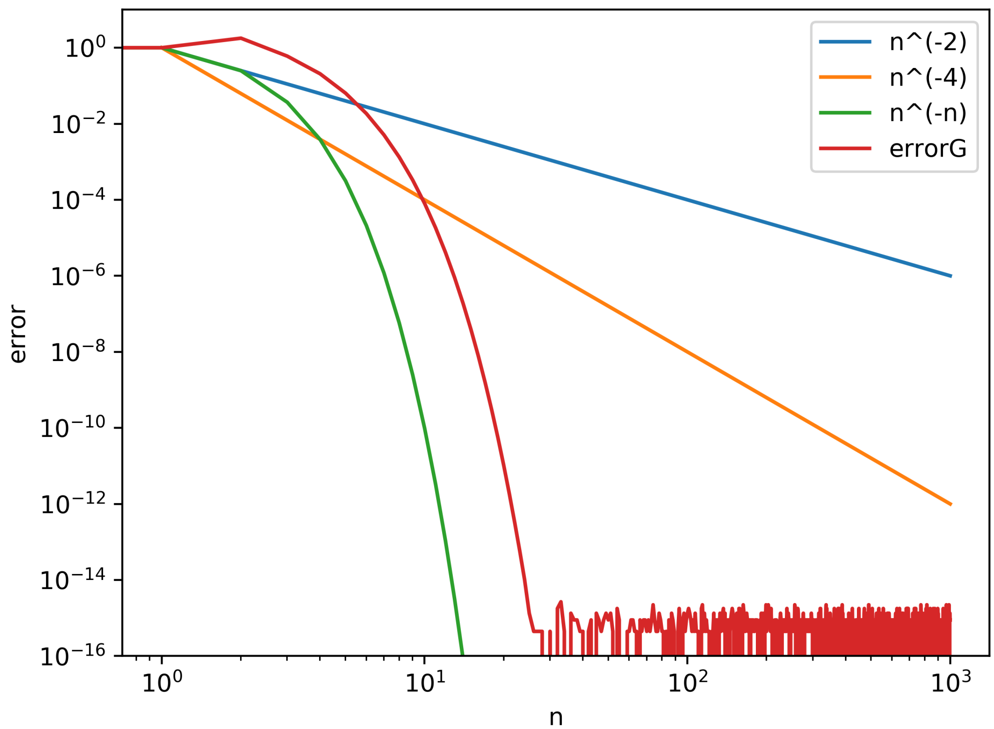

Figure 3: This figure shows the log-log plot of convergence of error for Gauss Quadrature used for evaluating I with $k = \pi$, showing comparison to quadratic and exponential convergence

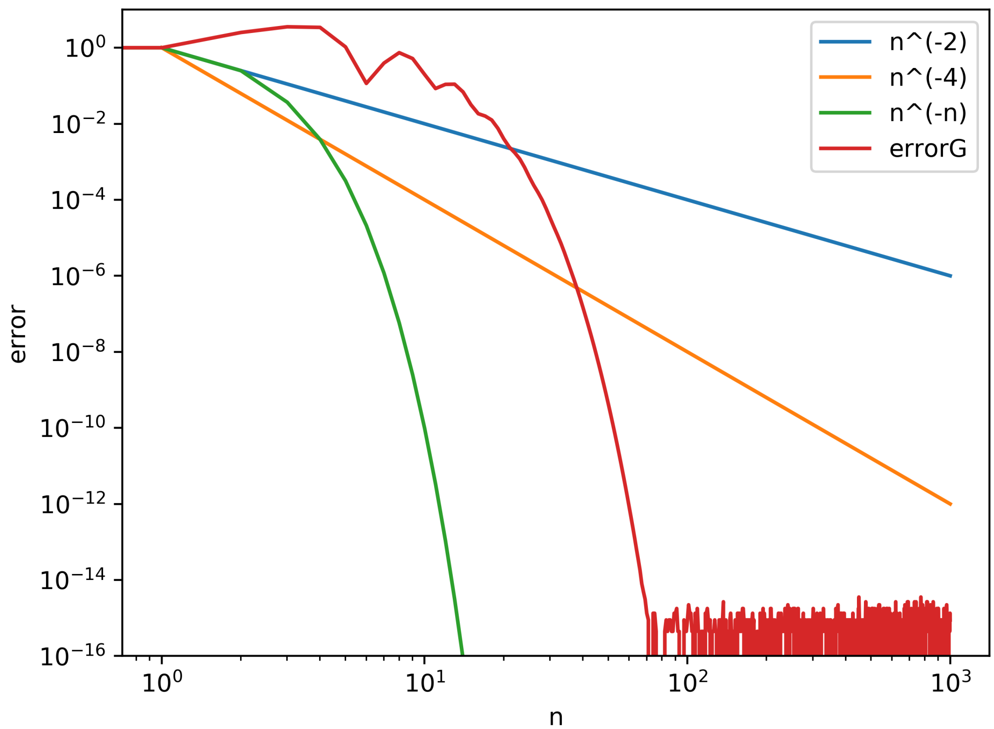

Figure 4: This figure shows the log-log plot of convergence of error for Gauss Quadrature used for evaluating I with $k = \pi^2$, showing comparison to quadratic and exponential convergence

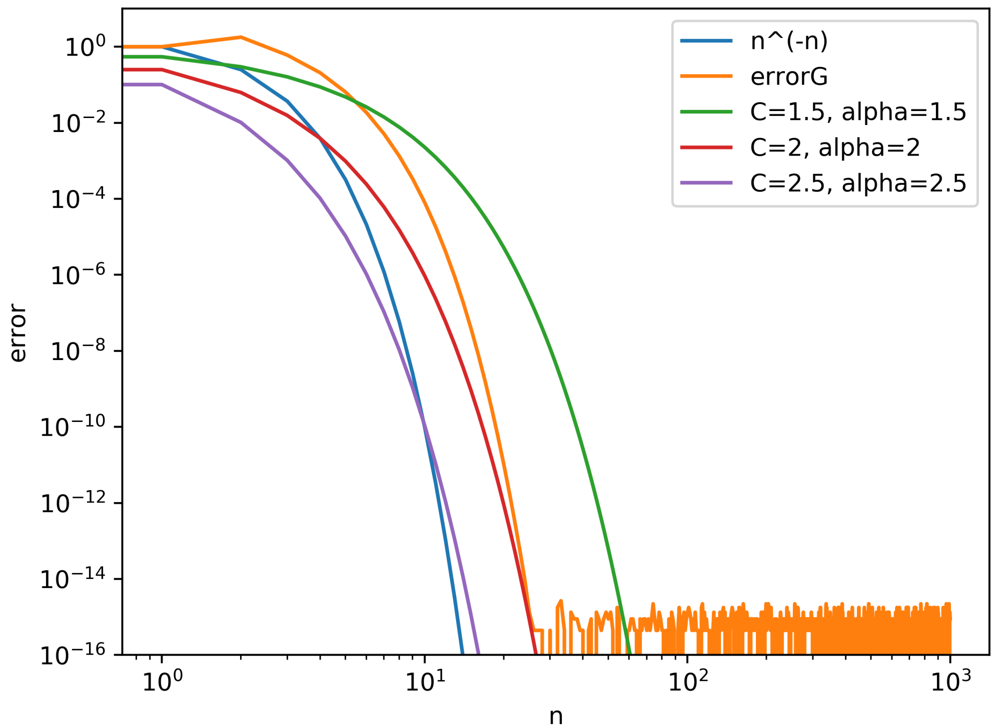

Figure 5: This figure shows the log-log plot of convergence of error for Gauss Quadrature used for evaluating I with $k = \pi$, showing comparison to different values of C and α in $\epsilon(n) = C^{\alpha n}$.

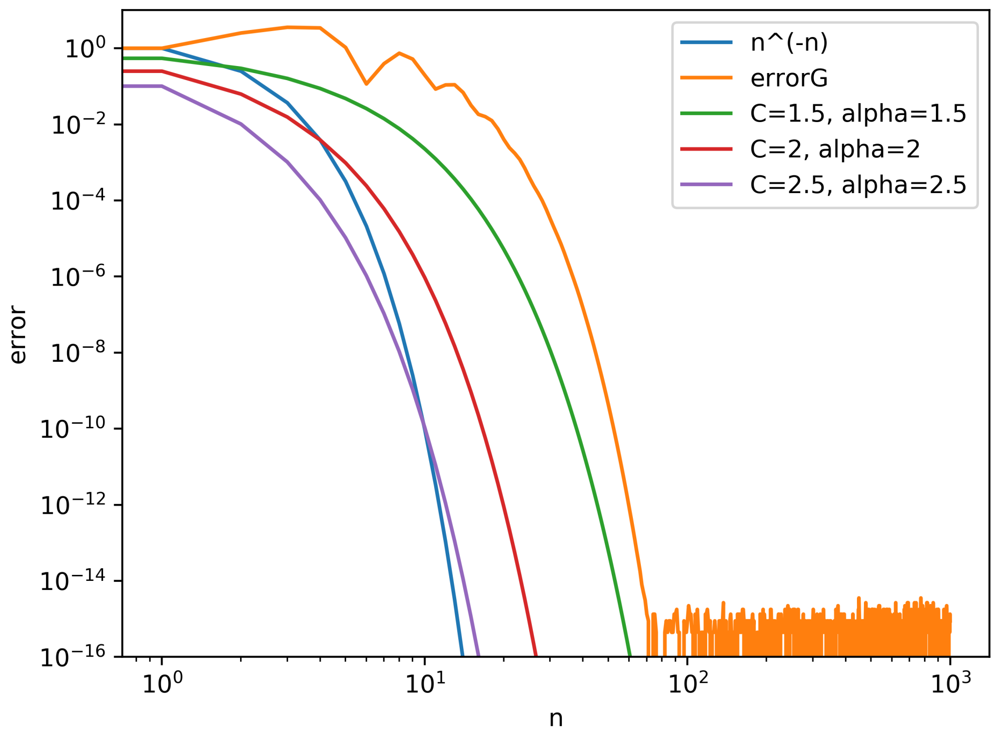

Figure 6: This figure shows the log-log plot of convergence of error for Gauss Quadrature used for evaluating I with $k = \pi^2$, showing comparison to different values of C and α in $\epsilon(n) = C^{\alpha n}$.