Solutions to Problem Set 2

Physics 305, Fall 2020

1. **One-dimensional Trapezoidal Method [15 Points]**

   - Write a Python function `trapezoidalRule(func, a, b, *P)` to compute the definite integral of the given function `func` between the given limits `a` and `b`. Use this function to compute the definite integral
   $$\int_0^1 xe^{-\alpha x}\,dx$$
   for $\alpha = 2$. [4 Points]
   - Run your code for $\mathbf{n} = \mathbf{50}, \mathbf{100}, \mathbf{200}, \mathbf{400}$. Evaluate the error in your approximation (by comparison with the analytic result), and plot the relative error as a function of **n** on a log-log plot, and compare with the expected order of convergence, which in this plot corresponds to a slope of $1/n^2$. [4 Points]
   - Find an approximate n such that the numerical answer is accurate to at least five significant figures. [2 Points]
   - Change step (iv) of the algorithm to **For** $i = 0, \ldots n$ **do steps 5 and 6.**. Does the order of convergence match the expected order ($O(1/n^2)$) or do you obtain a slope in your plot which is equal to -1? Provide an analytic explanation. [5 Points]

   ANSWER:

   A code example can be found in `trap1D_ps2_1.py`. When changing step (d) as described above, the code converges but only as $O(1/n)$, i.e., first-order convergence. This is demonstrated in Fig. 1. The reason for this is that in the sum we are double counting the contribution to the integral from $f(a)$ and $f(b)$, thus we have two additional terms in the expression for the integral, i.e., $hf(a) + hf(b) = h(f(a) + f(b))$, but these should not be there, and hence they contribute to the error. Since $f(a)$ and $f(b)$ are constants, these additional terms are $O(h) = O(1/n)$, which explains why the error goes down as $O(1/n)$.

2. **Two-dimensional Trapezoidal Method [10 Points]** Derive the trapezoidal method for double integrals in rectangular domains,where $x_i = a + ih_x,\ i = 0, 1, \ldots n$, with $h_x = (b - a)/n$, $y_j = c + jh_y,\ j = 0, 1, \ldots m$, with $h_y = (d - c)/m$, and where n and m can be either odd or even.

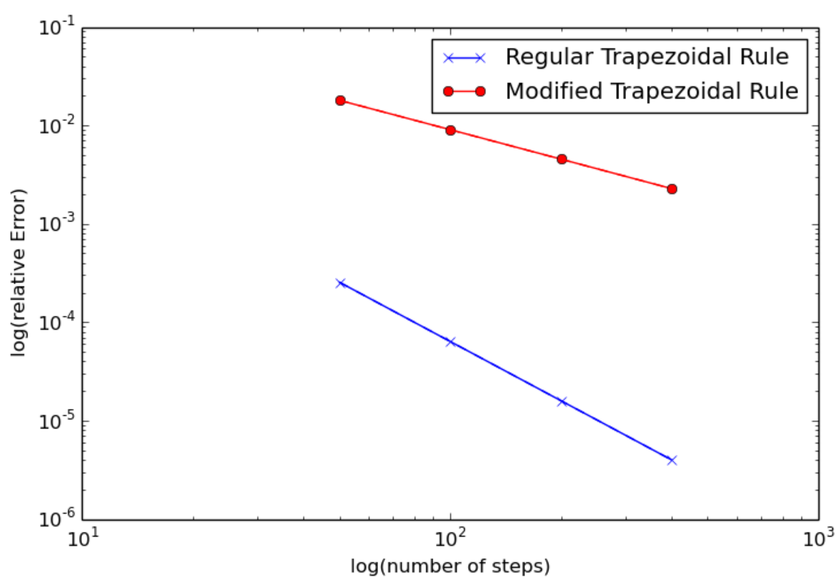

FIG. 1. Composite integration with incorrect trapezoidal method (error scaling like $1/n$), and the correct trapezoidal method (error scaling like $1/n^2$).

ANSWER:

The 1D composite trapezoidal rule is

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(a) + 2\sum_{i=1}^{n-1} f(x_i) + f(b)\right], \tag{1}$$

where $x_i = a + ih_x,\ i = 0, 1, \ldots n$, with $h_x = (b-a)/n$, and where n can be either even or odd. For the double integral we write

$$\int\int f(x,y)dxdy = \int_a^b \left(\int_c^d f(x,y)dy\right) dx \tag{2}$$

So, we first perform the innermost integral using the composite trapezoidal rule

$$\int_c^d f(x,y)dy = \frac{h_y}{2}\left[f(x,c) + 2\sum_{j=1}^{m-1} f(x,y_j) + f(x,d)\right], \tag{3}$$

where $y_j = c + jh_y,\ j = 0, 1, \ldots m$, with $h_y = (d-c)/m$. We can now plug Eq. (3) in Eq. (2), i.e.,

$$\int\int f(x,y)dxdy = \int_a^b \left(\frac{h_y}{2}\left[f(x,c) + 2\sum_{j=1}^{m-1} f(x,y_j) + f(x,d)\right]\right) dx \tag{4}$$

which we can rewrite as follows

$$\begin{aligned}\int\int f(x,y)dxdy =& \frac{h_y}{2}\left(\int_a^b f(x,c)dx + 2\sum_{j=1}^{m-1}\int_a^b f(x,y_j)dx + \int_a^b f(x,d)dx\right)\\ =& \frac{h_y}{2}\left(I_c + 2\sum_{j=1}^{m-1} I_j + I_d\right),\end{aligned} \tag{5}$$

where $I_c = \int_a^b f(x,c)dx,\ I_j = \int_a^b f(x,y_j)dx$, and $I_d = \int_a^b f(x,d)dx$. Now, we use the composite trapezoidal method to perform these 3 integrals, i.e.,

$$I_c = \int_a^b f(x,c)dx = \frac{h_x}{2}\left[f(a,c) + 2\sum_{i=1}^{n-1} f(x_i,c) + f(b,c)\right] \tag{6}$$

$$I_j = \int_a^b f(x,y_j)dx = \frac{h_x}{2}\left[f(a,y_j) + 2\sum_{i=1}^{n-1} f(x_i,y_j) + f(b,y_j)\right] \tag{7}$$

$$I_d = \int_a^b f(x,d)dx = \frac{h_x}{2}\left[f(a,d) + 2\sum_{i=1}^{n-1} f(x_i,d) + f(b,d)\right] \tag{8}$$

Substituing Eqs. (6)-(8) in Eq. (5) we find

$$\begin{aligned}\int\int f(x,y)dxdy =& \frac{h_y}{2}\left(I_c + 2\sum_{j=1}^{m-1} I_j + I_d\right)\\ =& \frac{h_x h_y}{4}\Bigg(f(a,c) + f(a,d) + f(b,c) + f(b,d) + 4\sum_{i=1}^{n-1}\sum_{j=1}^{m-1} f(x_i,y_j)\\ &+ 2\sum_{i=1}^{n-1} f(x_i,c) + 2\sum_{i=1}^{n-1} f(x_i,d) + 2\sum_{j=1}^{m-1} f(a,y_j) + 2\sum_{j=1}^{m-1} f(b,y_j)\Bigg)\end{aligned} \tag{9}$$

3. **Total charge of an equal charge electric dipole [15 Points]** An electric "dipole" consisting of two equal point charges q separated by a distance d has an electric field whose radial component far away from the source is given by

$$E_{\hat{r}} = \frac{1}{4\pi\epsilon_0}\left(\frac{2q}{r^2} + \frac{p\sin\theta\cos\phi}{r^3}\right). \tag{10}$$

where $p = qd$ is the magnitude of the dipole moment. Based on Gauss law's law the **total** charge inside a distant sphere of radius R is

$$Q = \epsilon_0 \int_{\mathcal{S}} E_{\hat{r}} R^2 \sin\theta d\theta d\phi = \frac{q}{4\pi}\int_0^{\pi}\int_0^{2\pi}\left(2 + \frac{d}{R}\cos\phi\sin\theta\right)\sin\theta d\theta d\phi \tag{11}$$

Build a code that implements the trapezoidal rule to perform the double integral appearing in the previous expression and find the total charge Q enclosed by the sphere assuming $d/R = 1/10$. Run your code for $n_\theta = n = n_\phi = m = 50, 100, 200, 400$. Does the value you obtain numerically converge to the expected result? If yes, at what order? Include a plot of the relative error vs n demonstrating the order of convergence in your solutions document.

ANSWER:

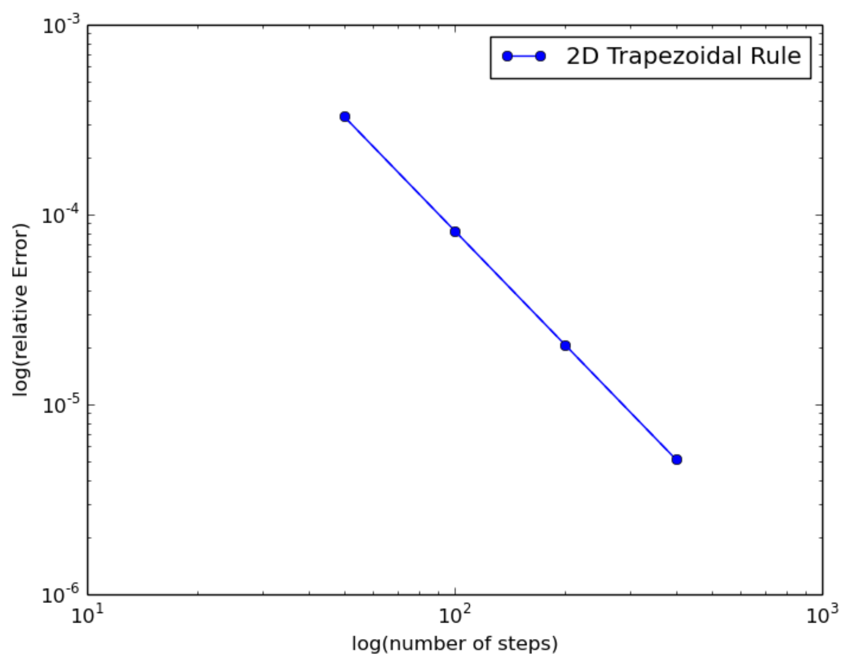

FIG. 2. Composite 2D integration with the trapezoidal method. Plotted is the relative error vs the number of sub-intervals in the ϕ and θ direction (n). The 2D composite trapezoidal method error scales like $1/n^2$, demonstrated by the $1/n^2$ curve shown which is parallel to the actual data.

A code example can be found in `trap2D_ps2_3.py`.

The exact answer for the total charge is $Q = 2q$. Thus, the double integral evaluates exactly to 8π. The composite 2D trapezoidal method converges to the value of 8π as shown in Fig. 2 which plots the relative error of the numerical integration with respect to the exact value of 8π. The order of convergence is 2, because the error curve is parallel to the line $1/n^2$.