Lab assignment #3: Gaussian Quadrature and Numerical Differentiation

Instructor: Nicolas Grisouard (nicolas.grisouard@utoronto.ca)
TA & Marker: Ahmed Rayyan (a.rayyan@mail.utoronto.ca)

Due Friday, October 1$^{\text{st}}$ 2021, 5 pm

Each room has a certain capacity, though we are not sure what it is.[1] So, first try to sign up for room 1. If it is full, sign up for room 2 and ask your partner to join you there if they are in room 1.

Room 1 (also for office hour) Ahmed Rayyan,
`https://gather.town/mIAKeWKElOnF4uL3/PHY407-AR`
PWD: `phy407ar`

Room 2 Nicolas Grisouard, `https://gather.town/app/2iGkhRu89WVOdW4X/phy407-ng-room1`
PWD: `phy407-ng-room1`

General Advice

- **Work with a partner!**
- Read this document and do its suggested readings to help with the pre-labs and labs.
- Ask questions if you don't understand something in this background material: maybe we can explain things better, or maybe there are typos.
- Specific instructions regarding what to hand out are written for each question in the form:

  THIS IS WHAT IS REQUIRED IN THE QUESTION.

  Not all questions require a submission: some are only here to help you. When we do though, we are looking for "C^3" solutions, i.e., solutions that are **C**omplete, **C**lear and **C**oncise.
- An example of **C**larity: make sure to label all of your plot axes and include legends if you have more than one curve on a plot. Use fonts that are large enough. For example, when integrated into your report, the font size on your plots should visually be similar to, or larger than, the font size of the text in your report.
- Whether or not you are asked to hand in pseudocode, you **need** to strategize and pseudocode **before** you start coding. Writing code should be your last step, not your first step. Test your code as you go, **not** when it is finished. The easiest way to test code is with `print()`

[1] The gather.town website says 25, but we have had more.

statements. Print out values that you set or calculate to make sure they are what you think they are. Practice modularity. It is the concept of breaking up your code into pieces that as independent as possible form each other. That way, if anything goes wrong, you can test each piece independently. One way to practice modularity is to define external functions for repetitive tasks. An external function is a piece of code that looks like this:

```
def MyFunc(argument):
    """A header that  explains the function
    INPUT:
    argument [float] is the angle in rad
    OUTPUT:
    res [float] is twice the argument"""
    res = 2.*argument
    return res
```

Place these functions in a separate file called e.g. `functions_labNN.py`, and call and use them in your answer files with:

```
import functions_labNN as fl  # make sure file is in same folder
ZehValyou = 4.
ZehDubble = fl.MyFunc(ZehValyou)
```

Computational background

Gaussian quadrature Section 5.6 of Newman provides a nice introduction to Gaussian quadrature. Example 5.2 on p. 170 gives you the tools you need to get started. The files referenced are `gaussint.py` and `gaussxw.py`. To use this code, you need to make sure that both files are in the same directory (so the import will work), or to know how to fetch them in different directories.

In Section 5.6.3 there's a discussion of errors in Gaussian quadrature, which are somewhat harder to quantify than for the previous methods we've seen. Equation (5.66) suggests that by doubling N we can get a pretty good error estimate:

$$\epsilon_N = I_{2N} - I_N. \tag{1}$$

Forward and Centred Differences The forward and centred approximations of a derivative are

$$\text{forward difference:} \quad \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x_i} \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}, \quad \text{and} \tag{2}$$

$$\text{centred difference:} \quad \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x_i} \approx \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}. \tag{3}$$

Physics background

The relativistic particle on a spring The energy of a relativistic particle, which is conserved, is given by

$$E = \frac{mc^2}{\sqrt{1 - v^2/c^2}} + \frac{1}{2}kx^2, \tag{4}$$

which can be rearranged to show that

$$v^2 = c^2\left[1 - \left(\frac{mc^2}{E - kx^2/2}\right)^2\right]. \tag{5}$$

Assume the particle started from rest from an initial position which we will call x_0. In this case $E = mc^2 + \frac{1}{2}kx_0^2$ and after rearranging terms we can write the following expression for the positive root:

$$v = \frac{\mathrm{d}x}{\mathrm{d}t} = c\left\{\frac{k\left(x_0^2 - x^2\right)\left[2mc^2 + k\left(x_0^2 - x^2\right)/2\right]}{2\left[mc^2 + k\left(x_0^2 - x^2\right)/2\right]^2}\right\}^{1/2} = g(x), \tag{6}$$

where $g(x)$ is a function of x. Notice that for $k\left(x_0^2 - x^2\right)/2 \ll mc^2$ we find $v \approx \sqrt{k\left(x_0^2 - x^2\right)}$, as expected for an energy conserving linear harmonic oscillator. For $k\left(x_0^2 - x^2\right)/2 \gg mc^2$, v approaches c but remains less than c.

Given (6), the period for the oscillation is given by four times the time taken for the particle to travel from $x = x_0$ to $x = 0$. Using separation of variables (see Example 5.10 in the text for a somewhat similar example),

$$T = 4\int_0^{x_0} \frac{\mathrm{d}x'}{g(x')}. \tag{7}$$

In the small and large amplitude limits described above, we expect T to approach $2\pi\sqrt{k/m}$ and $4x_0/c$, respectively. Because $g(x) \to 0$ as $x \to x_0^-$, the integral diverges in this limit and a fairly large number of points will be required for an accurate calculation.

Questions

1. **[45%] More on integrating functions**

   (a) In Lab 2, we evaluated the integral $I = \int_0^1 4(1+x^2)^{-1}\,\mathrm{d}x$ using the Trapezoidal and Simpson's rules, and compared with its actual value, which is π. We've now introduced Gaussian quadrature as a third method.

   i. Calculate the same integral with all three methods for a range of `N` slices/sample points between `N=8` and `N=2048`. *Note: you can just copy-and-paste a lot of what you did last week, or what is in the solution we provided (but mention which!). Having all methods on the same document helps with clarity of the results.*

   SUBMIT PRINTED OUTPUT AND EXPLANATORY NOTES.

   ii. Calculate the relative error compared to the true value, $I = \pi$, using these results and using eqn. (1), which requires you to do the calculation at 2`N` as well as at `N`.

   Plot the magnitude of the relative error on a log-log scale as a function of `N`, and describe the results, e.g., the relative size of the errors, the validity of the error estimate (1), etc.

   SUBMIT FIGURE(S), AND EXPLANATORY NOTES.

   (b) Diffraction of sound waves

i. Do Newman's Exercise 5.11 (p. 174). The two integrals for C and S listed in the exercise are called Fresnel integrals, and SciPy has an implementation of these functions.[2] Overlay your solution with the one obtained via SciPy to check that it is correct. Additionally, on a separate panel, plot the relative difference

$$\delta(x) = \frac{|I_{SP} - I_G|}{I_{SP}}, \tag{8}$$

where I_{SP} is the intensity field obtained with SciPy's implementation of the Fresnel integrals, and I_G is your own solution, which you obtained with the Gaussian quadrature.

SUBMIT YOUR PLOT AND EXPLANATORY NOTES, IF ANY.

ii. Now vary N from 3 to 50 and plot the maximum value of the relative difference $\max(\delta)$ as a function of N. You should have noticed in the previous question that δ gets rather large near the beginning of the x-range because there, we divide by very small values. To avoid this somewhat spurious effect, you may want to take the maximum of δ over a range where the signal is not negligible, say, for $x > -2$ or $x > 0$, as long as you clearly explain what you do.

Did we really need $N = 50$ points for the quadrature? What would have been an optimal value (there is no precise answer to this question, ballpark it)?

SUBMIT YOUR PLOT, YOUR CODE, EXPLANATORY NOTES IF ANY, AND ANSWER TO THE QUESTION.

(c) Now create a two dimensional picture of the intensity pattern of Q1b with the Gaussian quadrature method. Create an array of values of intensity over the range $-3 < x < 10$ and $1 < z < 5$ in the coordinates of the problem. Use filled colour contours, something like

```
plt.contourf(z, x, I, n)
```

or a pseudo-colour plot, as in

```
plt.pcolormesh(z, x, I)
```

To get a good resolution of the intensity, you will need to figure out how to choose all parameters and build arrays. Plot and describe qualitatively what happens as you go from $\lambda = 1$ m, to $\lambda = 2$ m, to $\lambda = 4$ m.

HAND IN YOUR CODE (SEPARATE FROM Q1(B)II), PLOTS AND WRITTEN ANSWERS.

2. **[40%] The period of a relativistic particle on a spring**

Using Gaussian quadrature, we will numerically calculate the period of the spring with the period given by eqn. (7), and see how it transitions from the classical to the relativistic case. The idea is to calculate T multiple times for a range of initial positions x_0 and assuming a mass of $m = 1$ kg and a spring constant $k = 12$ N/m.

[2] https://docs.scipy.org/doc/scipy/reference/generated/scipy.special.fresnel.html

(a) The first issue is accuracy of the solution. As x_0 gets smaller, the period should approach $2\pi\sqrt{m/k}$, which is the non-relativistic, linear (i.e., "boring") value. Check with the information given in the Physics background that $x_0 = 1$ cm indeed corresponds to the classical limit. Calculate the period for $N = 8$ and $N = 16$ for $x_0 = 1$ cm and compare this to the "boring" value. Estimate the fractional error for these two N's. To get a better sense of what affects the calculation, plot the integrands $4/g_k$ and the weighted values $4w_k/g_k$ at the sampling points. *Note: for each plot, you might want to combine the $N = 8$ and $N = 16$ cases for better readability.* Describe how these quantities behave as the x_0 limit of integration is approached. How do you think this behaviour might affect accuracy of the calculation?

HAND IN PLOTS AND WRITTEN ANSWERS.

(b) For a *classical* particle on a spring

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -kx, \tag{9}$$

what initial displacement $x_0 = x_c > 0$ for a particle initially at rest would lead to a speed equal to c at $x = 0$?

HAND IN YOUR WRITTEN ANSWER.

(c) For $N = 200$, what is your estimate of the percentage error for the small amplitude case? Now plot T as a function of x_0 for x_0 in the range $1\,\mathrm{m} < x < 10x_c$, and compare it to the relativistic and classical limits as suggested at the beginning of the problem.

HAND IN CODE FOR THE ENTIRE Q2, PLOTS AND WRITTEN ANSWERS.

3. **[15%] Numerical differentiation errors** Read section 5.10.2 in the textbook. Demonstrate that the optimum step size for forward difference differentiation schemes is indeed $\sqrt{C} \approx 10^{-8}$ by using the following example.

(a) Consider the function $f(x) = e^{-x^2}$. Using a forward difference scheme, numerically find the function's derivative at $x = 0.5$ for a range of h's from $10^{-16} \rightarrow 10^0$ increasing by a factor of 10 each step (so you should have 17 values for h with respective values of the derivative for each h value).

NOTHING TO SUBMIT (YET).

(b) Calculate the error in each derivative by comparing the value of the numerical derivative that you get to the analytic value. Take the absolute value of the error.

INCLUDE THE VALUES YOU FIND FOR Q3A AND 3B (ABSOLUTE VALUES ONLY FOR THE LATTER), SIDE-BY-SIDE.

(c) Plot the error as a function of step size on a log-log plot and show that the minimum is indeed at $\approx 10^{-8}$. Explain the shape of the curve by considering equation (5.91) in the text. When does the truncation error dominate? When does the rounding error dominate?

SUBMIT THE WRITTEN ANSWERS TO THESE QUESTIONS.

(d) Now implement a central difference scheme for the derivative and calculate the error for the same function. Plot the error in the central difference scheme on the same plot as your error for the forward difference scheme from Q3c. Concisely explain the key features of your plot. Does the central difference scheme **always** clearly beat the forward difference scheme in terms of accuracy?

SUBMIT YOUR CODE AND INCLUDE THE PLOT, WITH BOTH CURVES ON IT, AND ANSWERS TO THE QUESTIONS.