PHYS 361: Lab 7, Numerical Differentiation and Integration

Introduction

Forward, Backward, and Central Differencing Algorithms

All of these algorithms are based on the Taylor Expansion:

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + ... \quad (1)$$

The Taylor Series allows you to approximate the value of a function at some point x, using the known value at point a. If you keep the first team on the right-hand side of the equation, you are assuming you can estimate the next point using the slope of the line at $f(a)$ and drawing a straight line. You can add additional terms to improve your estimate because these consider the rate of change of the slope, the rate of change of the slope of the slope, and so on. If $f(x)$ were just a line, then the first term would be sufficient because all other terms would be zero.

You can use the first few terms of the Taylor Series to estimate the first derivative or rate of change of data (aka slope).

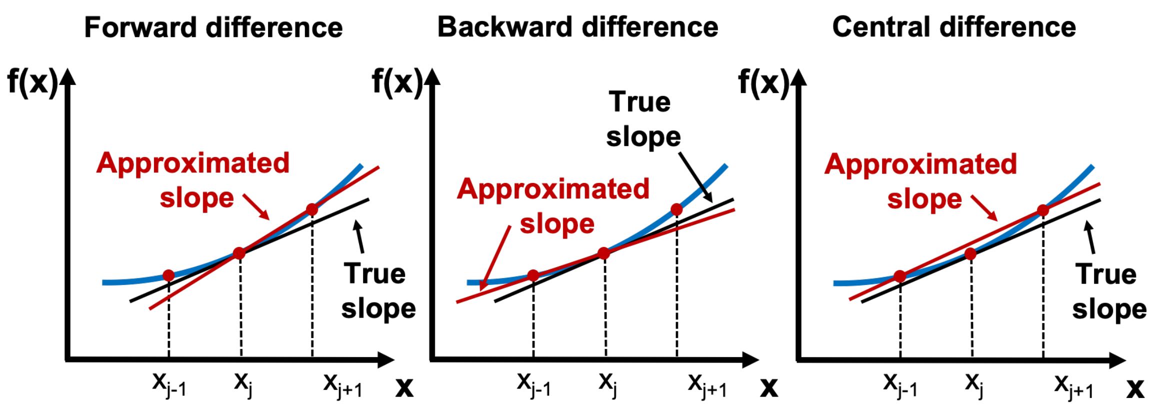

Figure 1: Finite Difference Schemes

The Forward Difference Formula uses the value of the function at x_j and $x_{j+1} = x_j + h$ to estimate the rate of change $f(x_j)$ at x_j.

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_j)}{h} \quad (2)$$

The Backward Difference Formula uses the value of the function at x_j and $x_{j+1} = x_j - h$ to estimate the rate of change $f(x_j)$ at x_j.

$$f'(x_j) = \frac{f(x_j) - f(x_{j-1})}{h} \quad (3)$$

The Central Difference Formula (assuming evenly spaced data) uses the value of the function the point x_{j-1} and $x_{j+1} = x_{j-1} + 2h$ to estimate the rate of change of $f(x_j)$ at a central point x_j.

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_{j-1})}{2h} \tag{4}$$

Riemann Sum Integration

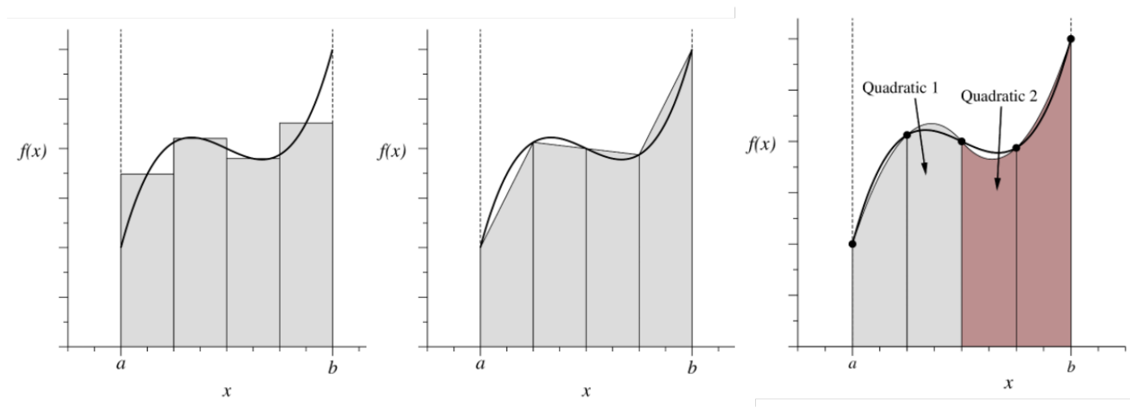

Figure 2: (left) Riemann Sum (middle) Trapezoid (right) Simpson's Rule

Riemann Sum integration allows you to estimate the integral (area under the curve) of a function or a data set by assuming you can estimate the area with rectangles.

$$Area \approx \sum_{i=1}^{N} h f(x_i) \tag{5}$$

The rectangles have a uniform width, h, and their height, $f(x_i)$, is given by the value of the function at the middle of the rectangle. The number of rectangles is defined by the limits of the integral and how wide the rectangles are, $N = \frac{b-a}{h}$.

Trapezoid Sum Integration

Trapezoid Sum integration improves on Riemann Sum integration because the sloped tops of the trapezoids follow the function more accurately. As shown in the lecture videos, you can simplify the sum of the area of each trapezoid with the following,

$$Area \approx \frac{1}{2}(f(a) + f(b) + 2\sum_{x=1}^{N-1} f(a + i \cdot h) \tag{6}$$

The trapezoids have a uniform width, h, and the height of each side is given by the value of the function. The number of trapezoids is defined by the limits of the integral and how wide the trapezoids are, $N = \frac{b-a}{h}$.

Simpson's Rule Integration

The last algorithm for numerical integration you learned about is called Simpson's Rule and is based on using polynomials for the top of our boxes that can recreate the curvature of the function. To derive this algorithm, we assumed a 2nd-order polynomial (quadratic),

$$P(u) = Au^2 + Bu + C \tag{7}$$

and found formulas for A, B, and C that depended on the width of the "box," h, and the values of the function at the ends and mid-points.

At the end of the lecture video, you were challenged to simplify the following formula with sums.

$$\begin{aligned} Area \approx \frac{1}{3}h(f(a) + 4f(a+h) + f(a+2h)) \\ +\frac{1}{3}h(f(a+2h) + 4f(a+3h) + f(a+4h))... \\ +\frac{1}{3}h(f(a+(N-2)h) + 4f(a+(N-1)h) + f(b)) \end{aligned} \tag{8}$$

This will make it easier to program!

Directions: Complete these problems by hand. Check them with the instructor before starting on the coding problems.

1. Evaluate the derivative of the function $f(x) = x^3$ by hand using the forward, backward, and central finite difference scheme at the points x=[2,3,4] and x=[2.75,3,3.25]. How do the results compare with the actual derivative evaluated at x=3?

2. Now, let's take the derivative of a data set. Let $x = [1.1, 1.2, 1.3, 1.4, 1.5]$ and $y = [0.6133, 0.7822, 0.9716, 1.1814, 1.4117]$. Estimate the rate of change of y with respect to x (e.g., dy/dx) by hand using the forward, backward, and central finite difference scheme at x=1.3.

3. Starting with the formula for the Taylor Expansion, derive a formula for numerically calculating the second derivative of a function or set of data. Your solution should use the substitution (combination of two equations) to eliminate the first derivative term (f'). Your final answer will be a "central differencing formula" because it estimates the second derivative at a central point (x_i) based on three points on the function calculated at three points (x_{i-1}, x_{i1}, x_{i+1}).

4. Take your central difference formula for the second derivative derived and use it to write a forward and backward difference formula for the second derivative. You can do this by substituting $i+1$ or $i-1$ for the i terms on the right-hand side of your formula *only*. The formulas for these differences won't be centered on x_i but will allow you to calculate the second derivative at the beginning and end of a data set.

5. Review your mid-week answer for simplifying the Simpson's Rule. Compare your answers with your classmates. Write your final solution below.

6. Calculate the following integral by hand, $\int_0^8 x^3 dx$ using,

   (a) The trapezoid rule with N=4.

   (b) The trapezoid rule with N=8.

   (c) Simpson's rule with N=4.

   (d) Compare each with the exact solution.

Directions: You should write a single script for each problem below. Put the number of the problem in the name of your script. Include all user-built functions at the bottom of your script. Make sure to include comments in your code and follow the format of a script used in the lectures (an example can be found on Canvas).

1. The position of an airplane at 5 seconds intervals as it accelerates on the runway is given in the following table:

$t(s)$	0	5	10	15	20	25	30	35	40
$x(t)$	0	20	53	295	827	1437	2234	3300	4658

   (a) Use the MATLAB user-defined function (`FirstDeriv`) to find the velocity of the airplane at each of the times in the data set. The program should calculate the derivative for the first two data points with the forward difference formula and the last two data points with the backward difference formula. At the mid-points, the program should calculate the derivative using the central difference scheme.

   (b) At the end of the same program, calculate the same derivative using MATLAB's built-in function `diff`.

2. Review the central, forward, and backward difference scheme for the second derivative your derived by hand.

   (a) Use it to write a user-defined function to evaluate the second derivative of a list of evenly spaced data. Call it `SecondDeriv`. It should use the forward, central, and backward difference scheme you derived for a second-order derivative to integrate a set of data, similar to what you did in the first problem.

   (b) Use your program to evaluate the velocity and acceleration of the space shuttle after launch based on the following *evenly* spaced data. At the end of the program, plot the altitude, vertical velocity, and vertical acceleration in three separate plots.

$t(s)$	0	10	20	30	40	50	60	70	80	90	100	110	120
$h(m)$	-8	241	1,244	2,872	5,377	8,130	11,617	15,380	19,872	25,608	31,412	38,309	44,726

3. Use a user-defined Simpson's rule function to solve the problems below. Do this in a single script file and report the results for each part of the problem using `fprintf`. Make sure what you print out makes sense and includes appropriate units.

   (a) The variation of gravitational acceleration, g, with altitude, y, is given by

   $$g = \frac{R^2}{(R+y)^2} g_0 \tag{9}$$

   where $R = 6371$ km is the radius of the Earth, and $g_0 = 9.81$ m/s^2. The change in gravitational potential energy, ΔU, is given by

   $$\Delta U = \int_0^h mgdy \tag{10}$$

   Determine the change in the potential energy of a satellite with a mass of 500 kg that is raised from the surface of the Earth to a height of 800 km.

   (b) The orbit of Pluto is elliptical, with a semi-major axis of $a = 5.9065 \times 10^9$ km and a semi-minor axis of $b = 5.7208 \times 10^9$ km. The perimeter of the ellipse can be calculated with the integral

   $$P = 4a \int_0^{pi/2} \sqrt{1 - k^2 sin^2\theta} d\theta \tag{11}$$

   where $k = \frac{\sqrt{a^2-b^2}}{a}$. Determine the distance Pluto travels in one orbit and calculate the average speed at which Pluto travels (in km/h) if one orbit takes about 248 year.

   (c) Do the same integrals using MATLAB's built-in function `integral`. Compare the results.

4. The Head Severity Index (HSI) measures the risk of head injury in a car crash. It is calculated with:

   $$HSI = \int_0^t [a(t)]^{2.5} dt \tag{12}$$

   where $a(t)$ is the acceleration normalized by dividing by 9.8 m/s^2 and t is time. In a car crash experiment the following acceleration of a dummy head was measured.

$t(ms)$	0	5	10	15	20	25	30	35	40	45	50	55	60
$a(m/s^2)$	0	3	8	20	33	42	40	48	60	12	8	4	3

   Copy the Reimann method code you wrote during the week to another file and change it so that it uses a user-defined function to calculate the integral of a tabular set of data using the Trapezoid method. In a single script file, compute the HSI from the data using your function and MATLAB's built-in function `trapz`. Compare the results.