Assignment 3

1. **Calculating asymptotic coefficients.** Finding the coefficients of higher order terms in an asymptotic expansion can become complicated. There can be expansions within expansions that have to be worked out. Here is an abstract example. Suppose we know

$$\begin{aligned} A(h) &= A_0 + hB_1(h) + h^2 B_2(h) + O(h^3) \\ B_1(h) &= C_0 + hC_1 + h^2 C_2 + O(h^3) \\ B_2(h) &= D_0 + hD_1 + O(h^2) \; . \end{aligned}$$

   Find formulas for the coefficients E_1, e_2, $\cdots$, so that

$$A(h) = A_0 + hE_1 + h^2 E_2 + O(h^3) \; .$$

   Note, this exercise gets more complicated (but not really harder) if you want to compute E_3 in terms of the C and D coefficients.

2. **Rectangle rule error expansion.**

   Suppose $f(x)$ is a smooth function and we want to compute

$$I = \int_0^1 f(x)\, dx \; .$$

   The rectangle rule (in notation from class) is

$$\widehat{I}(h) = \sum_{k=0}^{n-1} f(x_k)\Delta x \; .$$

   Find the coefficients

$$\widehat{I} - I = \Delta x I_1 + \Delta x^2 I_2 + \Delta x^3 I_3 + O(\Delta x^4) \; .$$

   The expansion coefficients I_1, I_2, and I_3 should be given in terms of values of f and its derivatives only at the endpoints $x = 0$ and $x = 1$. *Hint*: This involves summing the local error analysis and then approximating sums by integrals. For example, the leading term in the local error analysis is a power of Δx multiplying $f'(x_k)$. Summing over k, this is approximated (with an error term) by the integral of $f'(x)$, which is f itself evaluated at the endpoints. The idea of Exercise 1 probably also must be used.

3. **Reconstructing function values from cell averages.** Suppose you have *cell averages*

$$U_k = \frac{1}{\Delta x} \int_{B_k} f(x)\, dx \; .$$

We use the notation from class: $B_k = (x_{k-1}, x_k)$, with $x_k = a + k\Delta x$ and $b - a = n\Delta x$. In this context, bins or panels are often called *cells* or *zones*.

(a) Show that the cell average is a second order accurate estimate of the value of the function at the bin center. That is

$$U_k = f(x_{k-\frac{1}{2}}) + O(\Delta x^2) \; .$$

(b) Find a second order accurate estimate of $f(x_k)$ using U_k and U_{k+1}.

(c) Find a fourth order approximation to $f(x_{k-\frac{1}{2}})$ in terms of the k cell average and its two neighbors, U_k, U_{k-1}, and U_{k+1}.

4. **Simpson's rule.** Consider using the trapezoid rule with n and $2n$ points and using Richardson extrapolation to produce a fourth order method. Show that this has the form

$$I_k \approx \widehat{I}_k = \Delta x \left[\alpha f(x_{k-1}) + \beta f(x_{k-\frac{1}{2}}) + \alpha f(x_k) \right] \; .$$

Check explicitly that this integration rule, which is called *Simpson's rule*, is exact on constants, linears, quadratics, and cubics but not quartics. *Hint*: If you're looking for mathematical exactness or not, you can take $B_k = (-1, 1)$, $x_{k-1} = -1$, $x_k = +1$, which makes $\Delta x = 2$, and work with the monomials 1, x, $\cdots$, x^4. (why?)

5. **Accuracy validation, computational** Write a function that takes as arguments a, b, n, and f and produces an estimate of

$$\int_a^b f(x)\, dx \; .$$

Write two of these, one with the trapezoid rule and one with Simpson's rule. Write code to use this to do a *convergence study*, which is a table with columns for n with a sequence increasing by factors of 2 (e.g., 10, 20, 40, 80, etc.), for the error, and the ratio of errors with n and $2n$ points. Choose a range of n values so that at some point you see clear evidence of the order of accuracy (error ratios close to 4 and 16 respectively) and this pattern swamped by roundoff for larger n. Comment (in writing) on what n it takes to reach a given level of accuracy and in what range of n roundoff takes over. You may choose a, b and f as you want, but make sure that the problem is not trivial (e.g., f should not be a polynomial) and that you have a formula for the integral.

Table formatting: This exercise will be graded on the correctness of the results, and also on the quality of the table.

- Floating point numbers should be printed in a formatted way with a specified number of digits – all the same for each element of a given column but different for different columns. For example, the ratio can be in `f` format while the errors should be in `e` format. Choose the number of digits in a sensible way. Too many digits, as in `3.1415926535` if you don't need that much accuracy. The numbers in the table are for the boss, who will think you're thoughtless if you present a mass of digits she doesn't want/need to know (e.g. $\cdots$`926535`).
- The decimal points in each column should line up. This is almost automatic if you specify `e` or `f` format with a specified number of digits for each column.
- There should be column headings, with the numbers in the columns lining up under the column heading. It may take some trial and error to get the spacing in the for with headings right.

6. **Adaptive integrator**. The next assignment will ask you to write an adaptive integrator to pick the number of points needed to achieve a specific error for a specific function. This assignment is long enough already.