Numerical Methods; October–November 2023
Assignment 3
Due: Friday, 8 December 2023

Interpolation

You are given the following data:

x	y
0	1.0
1	2.0
2	1.0
3	0.5
4	4.0
5	8.0

▶ Use `scipy.interpolate.InterpolateUnivariateSpline` to fit a linear spline to these data. Now fit a quadratic spline. Next fit a cubic spline.

▶ Use Lagrange's method (`scipy.interpolate.lagrange`) to find the unique fifth-order polynomial that passes through the above six points.

▶ For the following functions, assume $x_0 = 0$, $x_1 = 0.6$, and $x_2 = 0.9$, construct interpolation polynomials to find $f(0.45)$, and report the absolute error:

1. $f(x) = \cos x$
2. $f(x) = \sqrt{1 + x}$
3. $f(x) = \ln(x + 1)$
4. $f(x) = \tan x$.

Nonlinear equations

▶ Solve the equation

$$\sin(\cos(\exp(x))) = 0$$

using the bisection method (`scipy.optimize.bisect`) using $(-1, 1)$ as your starting bracket. Report the result. Also report the value of $\sin(\cos(\exp(x)))$ at the root that you just obtained. Is it zero? If not, why not?

▶ Calculate the deriviative of $\sin(\cos(\exp(x)))$ using Wolfram Alpha. Then use the Newton-Raphson method (`scipy.optimize.newton`) with -1 as your initial guess to solve the above equation. Report the result. Next, repeat the procedure with -0.1 as your intial guess. Does the answer change? Why?

▶ If you do not specify the derivative, `scipy.optimize.newton` finds the root using the Secant method. Use it with -0.1 as your initial guess to solve the above equation.

▶ Using GSL, find the minimum of the Rosenbrock function

$$f(x, y) = (1 - x)^2 + 100\,(y - x^2)^2.$$

▶ Spend fifteen minutes reading the code for `scipy.optimize.newton` on GitHub. How does the Scipy authors' implementation of the Newton-Raphson algorithm compare with how you might have implemented this method?

Integration

▶ Compute

$$\int_0^1 \exp(x)dx$$

using

- the Trapezoidal rule (`scipy.integrate.trapezoid`)
- Simpson's rule (`scipy.integrate.simpson`)
- Romberg method (`scipy.integrate.romberg`)

▶ Use the Composite Trapezoidal Rule to compute the following integrals with the given number of evaluations:

1. $\int_1^2 x \ln x \,\mathrm{d}x, \quad n = 4$
2. $\int_0^2 \frac{2}{x^2+4} \,\mathrm{d}x, \quad n = 6$
3. $\int_0^{3\pi/8} \tan x \,\mathrm{d}x, \quad n = 8$

▶ Do the above exercise using the Composite Simpson's Rule.

▶ Use Romberg integration to compute $R_{3,3}$ for the following integrals:

1. $\int_1^{1.5} x^2 \ln x \,\mathrm{d}x$
2. $\int_0^1 x^2 e^{-x} \,\mathrm{d}x$
3. $\int_0^{\pi/4} (\cos x)^2 \,\mathrm{d}x$

▶ Spend fifteen minutes reading the code for `scipy.integrate.trapezoid` on GitHub.

Wrapping Up

▶ *Physical Review E* is a peer-reviewed journal published by the American Physical Society. Each issue of this journal has a section containing papers on Computational Physics. Spend 15 minutes on the Computational Physics section of Volume 108 Issue 4 (published October 2023) of this journal. What do the papers contain? Do they present new algorithms to solve certain physics problems? Do they present an analysis of these algorithms? Do you find a mention of any of the concepts that we learnt in our course in any of the papers?

▶ Do the same for Volume 493 (published 15 November 2023) of the *Journal of Computational Physics*, which is a peer-reviewed journal published by the Dutch company Elsevier.