CHEM1047 - Week 11 Lecture 1 – Numerical methods

☐ *Sections 20.5, 20.9 of Steiner, "The Chemistry Maths Book", 2nd edition.*

Not all functions are defined analytically, and not all differential equations have analytical solutions. The function may be the output of some very expensive instrument, measured only at specific points. The differential equation can be some magnetohydrodynamic monstrosity, painful even to look at. In these cases we must deal with functions and equations defined on discrete grids.

1. Numerical differentiation

The limit definition of the derivative

$$f'(x)=\lim_{\Delta x\to 0}\frac{f(x+\Delta x)-f(x)}{\Delta x} \tag{1}$$

suggests that the derivative of a function defined on a finite grid $\{x_1,...,x_N\}$ may be approximated:

$$f'(x_k)\approx\frac{f(x_{k+1})-f(x_k)}{x_{k+1}-x_k} \tag{2}$$

and the approximation will become better when the grid gets finer. Expressions like Equation (2) are called *finite difference approximations*. An important question is about their accuracy and the rate at which this accuracy improves when the grid gets finer.

Consider a grid with a fixed step Δx and the finite difference approximation in Equation (2):

$$f'(x_k)\approx\frac{f(x_k+\Delta x)-f(x_k)}{\Delta x} \tag{3}$$

We can use Taylor series to expand $f(x_k+\Delta x)$ around x_k:

$$f(x_k+\Delta x)=f(x_k)+f'(x_k)\Delta x+O(\Delta x^2) \tag{4}$$

Solving this for $f'(x_k)$ and replacing $f(x_k+\Delta x)$ with $f(x_{k+1})$ produces:

$$f'(x_k)=\frac{f(x_{k+1})-f(x_k)}{\Delta x}+O(\Delta x) \tag{5}$$

The accuracy of this *forward finite difference* approximation (called so because x_{k+1} is forward of x_k) therefore improves linearly when Δx is reduced.

Consider now the *central finite difference* approximation:

$$f'(x_k)\approx\frac{f(x_{k+1})-f(x_{k-1})}{2\Delta x}=\frac{f(x_k+\Delta x)-f(x_k-\Delta x)}{2\Delta x} \tag{6}$$

We need two Taylor series here, one for $f(x_k+\Delta x)$ and another for $f(x_k-\Delta x)$:

$$\begin{aligned}f(x_k+\Delta x)&=f(x_k)+f'(x_k)\Delta x+\frac{1}{2}f''(x_k)\Delta x^2+O(\Delta x^3)\\ f(x_k-\Delta x)&=f(x_k)-f'(x_k)\Delta x+\frac{1}{2}f''(x_k)\Delta x^2+O(\Delta x^3)\end{aligned} \tag{7}$$

Subtracting the two series and dividing the result by $2\Delta x$ yields:

$$f'(x_k)=\frac{f(x_{k+1})-f(x_{k-1})}{2\Delta x}+O(\Delta x^2) \tag{8}$$

This approximation to the derivative is superior to Equation (5) because its accuracy improves quadratically when the grid point spacing Δx is reduced.

Even higher accuracy methods exist. In practical calculations, it is important to make sure that the function is free of noise because noise makes numerical differentiation unstable.

2. Numerical methods for solving ODEs

Finite difference derivative expressions suggest a numerical method for solving differential equations. Consider a first-order ODE of the following general form:

$$\frac{d}{dt}f(t)=g\left[f(t),t\right] \tag{9}$$

Setting up a finite grid of time points $\{t_k\}$, setting $f_k=f(t_k)$, and replacing the derivative on the left hand side with a finite difference approximation yields:

$$\frac{f_{k+1}-f_k}{\Delta t}\approx g(f_k,t_k) \qquad \text{or} \qquad \frac{f_{k+1}-f_k}{\Delta t}\approx g(f_{k+1},t_{k+1}) \tag{10}$$

in which the left expression uses the value of $g\left[f(t),t\right]$ at the time point t_k, and the right expression uses $g(f_{k+1},t_{k+1})$. In the limit of $\Delta t\to 0$ these expressions are the same and identical to Equation (9). The left expression yields a simple formula for the sequence $\{f_k\}$:

$$f_{k+1}\approx f_k+g(f_k,t_k)\Delta t \tag{11}$$

If the initial condition f_0 is known, this formula permits the calculation of the entire sequence $\{f_k\}$ – the solution to the differential equation would be obtained numerically. The formula on the right side of Equation (10) also defines $\{f_k\}$, but an algebraic equation must be solved for f_{k+1} at every time step:

$$f_{k+1}\approx f_k+g(f_{k+1},t_{k+1})\Delta t \tag{12}$$

When these expressions are used to solve ODEs, Equation (11) is called *explicit Euler method* and Equation (12) is called *implicit Euler method*. Both are approximate, but the error may be made as small as necessary by making Δt smaller. The implicit method usually works better.

An accuracy analysis may be performed by looking at the Taylor expansion of $f(t_k+\Delta t)$ around t_k:

$$f(t_k+\Delta t)=f(t_k)+f'(t_k)\Delta t+O(\Delta t^2) \tag{13}$$

If we substitute the differential equation in the place of the derivative, and substitute the definition $f(t_k+\Delta t)=f_{k+1}$ on the left hand side, we obtain a more informative version of Equation (11):

$$f_{k+1}=f_k+g(f_k,t_k)\Delta t+O(\Delta t^2) \tag{14}$$

where the remainder now tells us that the error depends quadratically on the time step Δt. A great number of more sophisticated and accurate methods exist with errors of $O(\Delta t^3)$ or better.

Example: the differential equation describing the current in an electrical oscillator is

$$\frac{d^2}{dt^2}I(t)+\frac{R}{L}\frac{d}{dt}I(t)+\frac{1}{LC}I(t)=0$$

where R is the overall resistance of the circuit, L is inductance of the coil, and C is the capacitance of the capacitor. After assuming a discrete time grid with a step h and replacing all derivatives with central finite difference approximations, we obtain:

$$\frac{I(t_{k+1})-2I(t_k)+I(t_{k-1})}{h^2}+\frac{R}{L}\frac{I(t_{k+1})-I(t_{k-1})}{h}+\frac{1}{LC}I(t_k)=0$$

This is easily solved for $I(t_{k+1})$ with the result that a recurrently defined sequence is obtained for the next values of the current as a function of the previous values.

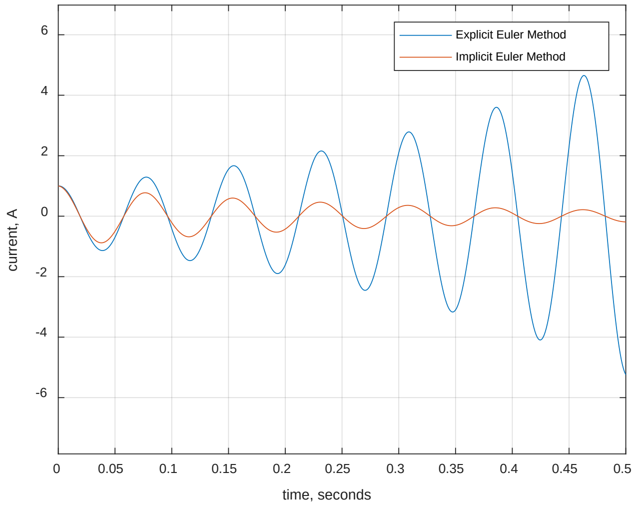

Figure 1. *Euler method solutions for a differential equation describing an electrical oscillator. The numerical instability of the explicit Euler method makes the solution accurate only up to about 25 ms.*

The implicit version of the same algorithm is in practice more accurate (Figure 1).

3. Numerical integration

A way of integrating numerically defined functions is suggested by the definition of Riemann integral:

$$\int_a^b f(x)\,dx \approx \sum_{k=0}^{N-1} f(x_k)\Delta x \tag{15}$$

The geometric meaning of this formula is illustrated in Figure 2 – it is an approximation to the area under the graph. The finer the grid, the more accurate the answer; a formal analysis of the Taylor series similar to the one we used for the derivatives yields the accuracy scaling estimate:

$$\int_a^b f(x)\,dx = \sum_{k=0}^{N-1} f(x_k)\Delta x + O[\Delta x] \tag{16}$$

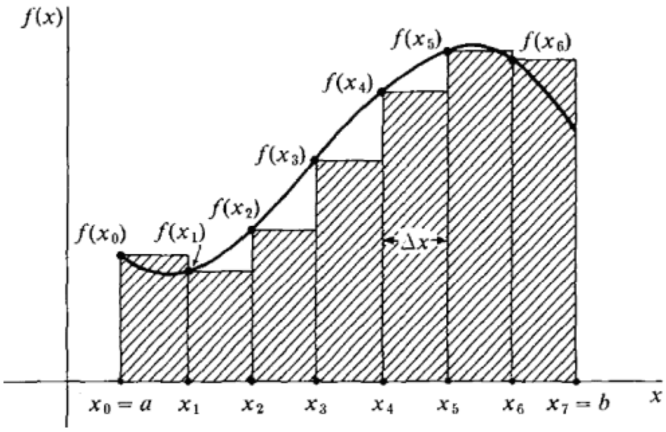

Figure 2. Graphical illustration of the rectangle integration rule. Function values are taken at the points located at the start of each interval.

Because the area is approximated as a sum of areas of individual rectangles, this procedure is called *rectangle rule*. More accurate methods are possible if the function is interpolated better.

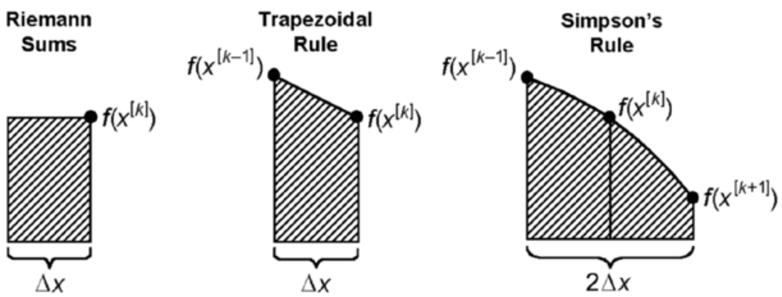

Figure 3. *Illustrations of the interpolation methods behind the rectangle rule (left), the trapezoidal rule (middle) and the Simpson rule (right).*

The most common methods are:

1. *Trapezoidal rule* (integrating a linear interpolant):

$$\int_a^b f(x)\,dx = \sum_{k=0}^{N-1} \frac{f(x_k) + f(x_{k+1})}{2}\Delta x + O\left[\Delta x^3\right] \tag{17}$$

2. *Simpson's rule* (integrating a quadratic interpolant):

$$\int_a^b f(x)\,dx = \sum_{k=0}^{N-1} \frac{1}{6}\left[f(x_k) + 4f\left(\frac{x_k + x_{k+1}}{2}\right) + f(x_{k+1})\right]\Delta x + O\left[\Delta x^5\right] \tag{18}$$

Even more sophisticated integration rules exist. They are outside the scope of this lecture, but all of them are based on the same general idea – an interpolant is built and integrated.