2 Finite difference methods

This week we discuss how to perform approximated calculus using small finite difference in place of a formal limit to 0. Before starting you should ensure that you're comfortable with the following Taylor expansions:

$$f(x+\delta x) \approx f(x) + f'(x)\delta x \tag{1a}$$

$$f(x+\delta x) \approx f(x) + f'(x)\delta x + f''(x)\frac{\delta x^2}{2} \tag{1b}$$

$$f\big(x+\frac{\delta x}{2}\big) \approx f(x) + f'(x)\frac{\delta x}{2} + f''(x)\frac{\delta x^2}{8} \tag{1c}$$

$$f(x+\delta x, y+\delta y) \approx f(x,y) + \left.\frac{\partial f}{\partial x}\right|_{x,y}\delta x + \left.\frac{\partial f}{\partial y}\right|_{x,y}\delta y \tag{1d}$$

2.1 Differentiation

We can approximate a derivative by essentially rearranging Eq. (1a). This yields the forward and backward derivatives:

$$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_x \equiv f'(x) \approx \frac{f(x+\delta x) - f(x)}{\delta x}, \tag{2a}$$

$$f'(x) \approx \frac{f(x) - f(x-\delta x)}{\delta x}, \tag{2b}$$

which have errors of order $\mathcal{O}(\delta x^2)$.

We can do better by using a midpoint derivative:

$$f'(x) \approx \frac{f(x+\frac{\delta x}{2}) - f(x-\frac{\delta x}{2})}{\delta x}. \tag{3}$$

The error in the midpoint derivative is found by subtracting two versions of Eq. (1c) with $\pm\delta x$

$$f\big(x+\frac{\delta x}{2}\big) \approx f(x) + \frac{\delta x}{2}\,f'(x) + \frac{\delta x^2}{8}\,f''(x), \tag{4a}$$

$$f\big(x-\frac{\delta x}{2}\big) \approx f(x) - \frac{\delta x}{2}\,f'(x) + \frac{\delta x^2}{8}\,f''(x), \tag{4b}$$

$$\implies f'(x) \approx \frac{f\big(x+\frac{\delta x}{2}\big) - f\big(x-\frac{\delta x}{2}\big)}{\delta x}, \tag{4c}$$

showing a cancellation of the second derivative curvature term, thus giving an error of order $\mathcal{O}(\delta x^3)$.

2.2 Integration

The other important operation in calculus is integration. We will understand this as simply achieving the function $f(x)$ from its derivative $f'(x)$, and will make reference to the geometric interpretation of this is as area under a curve. In practice we find an integrated function by building in small increments, achieving an $f(x + \delta x)$ from given value of $f(x)$. This means a starting value must be provided, corresponding to the $+C$ that we so frequently omit.

Again the simplest integration is by rearranging Eq. (1a):

$$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_x \equiv f'(x) \approx \frac{f(x+\delta x) - f(x)}{\delta x} \implies f(x+\delta x) \approx f(x) + f'(x)\,\delta x. \tag{5}$$

We can think of this as adding many rectangles to approximate the area under the curve. We can recast it as a definite integral by using the formula n times at intervals of δx spanning a total interval from a to b:

$$\int_a^b f'(x)\,\mathrm{d}x \approx \sum_{i=0}^{n-1} f'(a + i\delta x)\,\delta x, \text{ with } \delta x = \tfrac{b-a}{n}. \tag{6}$$

Since the error in each estimate is $\mathcal{O}(\delta x^2) \sim \mathcal{O}(1/n^2)$, and there are n of them, the total error is $\mathcal{O}(1/n)$.

By expanding to second order we can improve this. However, we in principle don't know the form of $f''(x)$, and hence we use an approximate derivative to evaluate the curvature:

$$f(x+\delta x) \approx f(x) + f'(x)\delta x + f''(x)\frac{\delta x^2}{2}, \tag{7a}$$

$$f''(x) \equiv g'(x) \approx \frac{g(x+\delta x) - g(x)}{\delta x} = \frac{f'(x+\delta x) - f'(x)}{\delta x}, \tag{7b}$$

$$\implies f(x+\delta x) \approx f(x) + \Big[f'(x+\delta x) + f'(x)\Big]\frac{\delta x}{2}. \tag{7c}$$

This is known as the trapezoidal rule, and is thought of as adding a rectangle with a small triangle on top. Again, we recast this as a definite integral:

$$\int_a^b f'(x)\,\mathrm{d}x \approx f'(a)\,\frac{\delta x}{2} + \sum_{i=1}^{n-1} f'(a + i\delta x)\,\delta x + f'(b)\frac{\delta x}{2}\,. \tag{8}$$

Since the error on the individual estimates is now $\mathcal{O}(\delta x^3)$, the total error is $\mathcal{O}(1/n^2)$.

The above approach can be improved somewhat by avoiding two function evaluations. The intuition is that the average of gradients between x and $x + \delta x$ is approximately the gradient at the midpoint $x + \delta x/2$. We confirm this intuition by combining (1c) with (7a), which gives

$$f(x+\delta x) \approx f(x) + f'\big(x + \frac{\delta x}{2}\big)\delta x. \tag{9}$$

The difference is only $\mathcal{O}(\delta x^3)$, which is anyway the order of the error, so this is formally equally accurate. It is called the mid-point rule, and gives a definite integral

$$\int_a^b f'(x)\,\mathrm{d}x \approx \sum_{i=0}^{n-1} f'(a + (i + \tfrac{1}{2})\delta x)\,\delta x. \tag{10}$$

Finally, examining the error terms of the trapezoidal and mid-point rules, we find that both the δx^2 and δx^3 terms of the mid-point rule are a factor of 2 smaller, and of opposite sign, to the trapezoidal rule. Therefore, combining them in $\frac{2}{3}$ and $\frac{1}{3}$ proportion, gives an error term of δx^4:

$$f(x+\delta x) \approx f(x) + \frac{1}{6}f'\big(x\big)\delta x + \frac{2}{3}f'\big(x+\frac{\delta x}{2}\big)\delta x + \frac{1}{6}f'\big(x+\delta x\big)\delta x. \tag{11}$$

It is known as Simpson's rule, and gives a definite integral

$$\int_a^b f'(x)\,\mathrm{d}x \approx \frac{1}{6}\left[f'(a) + 4\sum_{i=0}^{n-1} f'(a+(i+\tfrac{1}{2})\delta x) + 2\sum_{i=1}^{n-1} f'(a+i\delta x) + f'(b)\right]\delta x \tag{12}$$

with total error $\mathcal{O}(1/n^4)$.

2.3 Solving ODEs

Solving an ODE is, in broad strokes, solving an integral. Consider for example a geometric interpretation that the distance travelled is the area under the velocity-time curve. There is however one big difference in solving ODEs, which is the influence the system has on its own evolution. Consider for example a mass on a spring which will change velocity based on how far the mass has travelled away from the equilibrium point. We will therefore expand the previous ideas on integration to allow for a simultaneous time integration of many variables that all influence one another. We will end up with a very popular form for solving ODEs known as Runge-Kutta (RK) methods.

To start, consider a simple case of a system with one variable x and time t. We know the gradient function

$$\frac{\mathrm{d}x}{\mathrm{d}t} \equiv \dot{x} = f(t,x). \tag{13}$$

Hopefully it is clear that one (inaccurate) method is to simply use

$$x(t+\delta t) \approx x(t) + f(t,x)\delta t \tag{14}$$

where no complications arise from the system's own dependence on x.

It is at second order we see the system dependence and unpack a total derivative into two partial derivatives.

$$\begin{aligned}
x(t+\delta t) &\approx x(t) + \dot{x}\delta t + \ddot{x}\frac{\delta t^2}{2} \\
&= x(t) + f(t,x)\delta t + \frac{\mathrm{d}f}{\mathrm{d}t}\frac{\delta t^2}{2} \\
&= x(t) + f(t,x)\delta t + \left[\frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\dot{x}\right]\frac{\delta t^2}{2} \\
&= x(t) + f(t,x)\delta t + \left[\frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}f(t,x)\right]\frac{\delta t^2}{2}
\end{aligned} \tag{15}$$

We now take inspiration from our midpoint integration method and evaluate f at the mid-point of both time and state. The midpoint in state is defined as the hypothetical state of the system after a half step using Eq. (14):

$$f\left(t+\frac{\delta t}{2},\, x+f(t,x)\frac{\delta t}{2}\right) \approx f(t,x) + \frac{\partial f}{\partial t}\frac{\delta t}{2} + \frac{\partial f}{\partial x}f(t,x)\frac{\delta t}{2} \tag{16}$$

We now compare the terms in Eq. 15 and Eq. 16 to write

$$x(t+\delta t) \approx x(t) + f\left(t + \frac{\delta t}{2},\, x + f(t,x)\frac{\delta t}{2}\right)\delta t \tag{17}$$

This method is called RK2, owing to its initial perturbation order, and thus its accuracy. A more conventional and more easily generalisable form to write the equations is by naming the intermediate states k_n as follows:

$$k_1 \equiv f(t,x)\delta t, \tag{18a}$$

$$k_2 \equiv f\big(t + \frac{\delta t}{2},\, x + \frac{k_1}{2}\big)\delta t, \tag{18b}$$

$$x(t+\delta t) = x(t) + k_2. \tag{18c}$$

Note that in the case that f does not depend explicitly on x, $f(t,x) = f(t)$, this is identical to the midpoint integration method.

Hopefully the derivation of RK2 has emphasised that deriving higher orders will be quite painful. Thus we will state the results for the most popular algorithm, RK4, with no derivation. Furthermore we will generalise to an entire vector of state variables $\vec{x} = (x_1, x_2, ...)^{\mathrm{T}}$:

$$\vec{k_1} \equiv \vec{f}(t,\, \vec{x})\delta t, \tag{19a}$$

$$\vec{k_2} \equiv \vec{f}\left(t + \frac{\delta t}{2},\, \vec{x} + \frac{\vec{k_1}}{2}\right)\delta t, \tag{19b}$$

$$\vec{k_3} \equiv \vec{f}\left(t + \frac{\delta t}{2},\, \vec{x} + \frac{\vec{k_2}}{2}\right)\delta t, \tag{19c}$$

$$\vec{k_4} \equiv \vec{f}(t + \delta t,\, \vec{x} + \vec{k_3})\delta t, \tag{19d}$$

$$\vec{x}(t+\delta t) = \vec{x}(t) + \frac{1}{3}\left(\frac{\vec{k_1}}{2} + \vec{k_2} + \vec{k_3} + \frac{\vec{k_4}}{2}\right). \tag{19e}$$

The RK4 method boasts an error term of only $\mathcal{O}(\delta t^5)$ per step, so $\mathcal{O}(1/n^4)$ over a finite range of t. It is often chosen as a good middle ground between accuracy and speed. Note again that in the case that $\vec{f}$ does not depend explicitly on $\vec{x}$, RK4 is identical to the Simpson's rule integration method.

One final step we must take to solve physical ODEs is to decouple second order differential equations into two separate coupled first order equations. This is simply done by considering velocity as its own *independent* variable. Consider a system following $\ddot{x} = f(t,x)$. We can decompose this as

$$\dot{x} = v, \tag{20}$$

$$\dot{v} = f(t,x). \tag{21}$$

With all these techniques in place we can solve many of the equations we face in physics!