

Derivation of finite difference equations

Consider a grid of equally spaced points x_n with spacing Δx . If we are given the value of a function $y = f(x)$ at a grid point, and given the first derivative df/dx , we could find the value of the function at the next grid point using Euler's method, which uses *only the first term* in the Taylor expansion:

$$f(x_{n+1}) = f(x_n) + \Delta x \frac{df(x_n)}{dx}$$

In the region between the grid points, the first derivative may change, thus we make a small error proportional to both $(\Delta x)^2$ and the second derivative. Below, we will *keep the second derivative* to improve the accuracy of our methods.

Numerical integration: finding the function from the first derivative

Let's look at the Taylor expansion to second order, about the point x_n , and allow the next point to be at either at $x + \Delta x$ or at $x - \Delta x$:

$$f(x_n \pm \Delta x) = f(x_n) \pm \Delta x \frac{df(x_n)}{dx} + \frac{1}{2} \Delta x^2 \frac{d^2 f(x_n)}{dx^2}$$

Take the version of the equation with the + sign and subtract the version of the equation with the minus sign, and rearrange to find:

$$f(x_n + \Delta x) - f(x_n - \Delta x) = -2\Delta x \frac{df(x_n)}{dx}$$

$$\frac{df(x_n)}{dx} = \frac{1}{2\Delta x} [f(x_n + \Delta x) - f(x_n - \Delta x)]$$

Note that the two contributions of the second derivative term have cancelled. Any error that we have made must come from the next term in the expansion, proportional to $(\Delta x)^3 d^3 f(x)/dx^3$. This term is going to be small if Δx is sufficiently small.

If the first derivative increases in going from x_n to $x_{n+1} = x_n + \Delta x$, and if the second derivative isn't changing much, the first derivative must *decrease* if I go backward from x_n to $x_n - \Delta x$. If I average the first derivative calculated on the left side of x_n with the first derivative on the right side of x_n , then the two errors from the second derivative are of opposite sign and cancel. The last equation above is exactly the average of the derivative from the left side and the derivative from the right side.

Example: find E_n from $-\text{grad } \phi_n$:
$$E(x_n) = \frac{-1}{2\Delta x} [\phi(x_{n+1}) - \phi(x_{n-1})]$$

Now let's replace Δx by $\Delta x/2$, and rewrite the last equation before the example:

$$\frac{df(x_n)}{dx} = \frac{1}{\Delta x} [f(x_{n+1/2}) - f(x_{n-1/2})]$$

where $n+1/2$ means the point half way between the grid points x_n and x_{n+1} .

Now apply this equation at the point $x_{n+1/2}$ and get

$$f(x_{n+1}) = f(x_n) + \Delta x \frac{df(x_{n+1/2})}{dx} \quad \text{The midpoint method of integration}$$

In the above equation, there is no second order derivative term because that term cancelled out in the derivation. Thus given $f(x)$ and the derivative *half way* to the next point, I can find $f(x)$ at the next point with no error from the second derivative term. This is an improvement upon Euler's method.

Example: find $E_{n+1/2}$ from $-\text{grad } \phi$:
$$E(x_{n+1/2}) = \frac{-1}{\Delta x} [\phi(x_{n+1}) - \phi(x_n)]$$

Example: find ϕ from E :
$$\phi(x_{n+1}) = \phi(x_n) - \Delta x \cdot E(x_{n+1/2})$$

Finding the second derivative given the function

If we are given the function and want to find the second derivative, we can do that by returning to the Taylor expansion above and *adding* the equation for $f(x_n - \Delta x)$ to the equation for $f(x_n + \Delta x)$ to obtain

$$f(x_n + \Delta x) + f(x_n - \Delta x) = 2f(x_n) + \Delta x^2 \frac{d^2 f(x_n)}{dx^2}$$

In the addition, the first order terms cancelled. We can rearrange to get

$$\frac{d^2 f(x_n)}{dx^2} = \frac{1}{(\Delta x)^2} [f(x_n + \Delta x) - 2f(x_n) + f(x_n - \Delta x)]$$

We can rewrite this in more compact notation

$$\frac{d^2 f_n}{dx^2} = \frac{1}{(\Delta x)^2} [f_{n+1} - 2f_n + f_{n-1}] = \frac{2}{(\Delta x)^2} [\frac{1}{2}(f_{n+1} + f_{n-1}) - f_n]$$

The last version of the equation is written to make the following point. If the value of f_n is equal to the average of the values at the two neighboring points, $[f_{n+1} + f_{n-1}] / 2$, the second derivative is zero. In this case we have a straight line. If the midpoint of a line segment is higher than the end points, the second derivative is negative (curving downward), and if the midpoint is lower than the end points, the second derivative is positive (curving upward).

The Runge Kutta method

Write the Taylor expansion about the point at n using half a grid spacing:

$$f(x_{n\pm 1/2}) = f(x_n) \pm \frac{\Delta x}{2} \frac{df(x_n)}{dx} + \frac{1}{2} \left(\frac{\Delta x}{2} \right)^2 \frac{d^2 f(x_n)}{dx^2} \pm \frac{1}{6} \left(\frac{\Delta x}{2} \right)^3 \frac{d^3 f(x_n)}{dx^3} + \dots$$

Subtract the version of the equation with the minus sign from the equation with the plus sign:

$$f_{n+1} = f_n + \Delta x \frac{df_{n+1/2}}{dx} + \frac{1}{3} \left(\frac{\Delta x}{2} \right)^3 \frac{d^3 f_{n+1/2}}{dx^3}$$

where n has been everywhere replaced by n + 1/2 so that the equation is symmetric about n + 1/2.

The $(\Delta x)^2$ and $(\Delta x)^4$ terms cancelled. We don't know the third derivative, but it is the second derivative of df/dx and we know how to find second derivatives. Using our result for the second derivative that we derived three equations previously, we get

$$\frac{d^3 f_{n+1/2}}{dx^3} = \left(\frac{2}{\Delta x} \right)^2 \left[\frac{df_{n+1}}{dx} - 2 \frac{df_{n+1/2}}{dx} + \frac{df_n}{dx} \right]$$

The third derivative is found by evaluating the first derivative three times: at n, at n+1/2, and at n+1. Put this form of the third derivative into the previous equation and rearrange to get

$$\begin{aligned} f_{n+1} &= f_n + \Delta x \frac{df_{n+1/2}}{dx} + \frac{1}{6} \Delta x \left[\frac{df_n}{dx} - 2 \frac{df_{n+1/2}}{dx} + \frac{df_{n+1}}{dx} \right] \\ &= f_n + \frac{1}{6} \Delta x \left[\frac{df_n}{dx} + 4 \frac{df_{n+1/2}}{dx} + \frac{df_{n+1}}{dx} \right] \end{aligned}$$

This is the basis for the Runge Kutta method, but is not the complete story. Suppose our derivative df/dx is both a function of x and of $y = f(x)$. Then we must evaluate the derivative using the correct values for y at n+1/2 and n+1. A more detailed analysis gives this result:

$$\begin{aligned} f_n &= f_{n-1} \\ &+ \frac{1}{6} \Delta x \left[\frac{df(x_n, y_n)}{dx} + 2 \frac{df(x_{n+1/2}, y + \frac{1}{2} dy_a)}{dx} + 2 \frac{df(x_{n+1/2}, y + \frac{1}{2} dy_b)}{dx} + \frac{df(x_{n+1}, y + dy_c)}{dx} \right] \end{aligned}$$

where the three increments in y that we have used are

$$dy_a = \Delta x \frac{df(x_n, y_n)}{dx} \quad dy_b = \Delta x \frac{df(x_{n+1/2}, y_n + \frac{1}{2} dy_a)}{dx} \quad dy_c = \Delta x \frac{df(x_{n+1/2}, y_n + dy_b)}{dx}$$

This reduces to the simpler equation when df/dx is not a function of $y = f(x)$.

It is not uncommon to have a derivative which is the function of the dependent variable. For example, consider a block sliding on a plane with friction. The equation of motion is $m dv/dt = -\alpha v$ where α is a coefficient. The derivative is a function of v, not a function of t. That means we have to extrapolate the value of v to the next grid point in order to find the derivative at the next grid point. The increments dy_a , dy_b , and dy_c above are the extrapolations of the dependent variable. The extrapolation dy_a is made with the derivative at the left end of the interval from y_n to $y_{n+1/2}$, and the extrapolation dy_b is made with the derivative from the right end of the interval. The derivatives from the two different y values are averaged and this average replaces the $4 df_{n+1/2}/dx$ that appears in

the previous formula.

Mathcad 's Runge Kutta routine

The Mathcad Resource Center on the Help menu gives the following equations for Runge Kutta integration:

$$k_1 := h \cdot D(x_0, y^{(0)})$$

h is the same as our Δx .

$$k_2 := h \cdot D\left(x_0 + \frac{h}{2}, y^{(0)} + \frac{k_1}{2}\right)$$

k_2 , k_3 , and k_4 are our dy_a , dy_b , and dy_c above.

$$k_3 := h \cdot D\left(x_0 + \frac{h}{2}, y^{(0)} + \frac{k_2}{2}\right)$$

$$k_4 := h \cdot D(x_0 + h, y^{(0)} + k_3)$$

$$y^{(1)} := y^{(0)} + \left(\frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6}\right)$$

This determines the next y value from the present y value. Here, y is a vector of values that might be the x , y , and z coordinates of a particle.