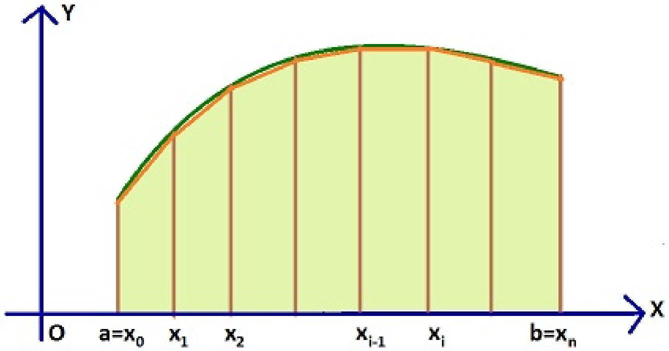
EE2-8C Mathematics
Numerical Analysis of Differential Equations

Introductory Exercise:Trapezoidal Rule I

Not every integral has an exact solution. To approximate a solution we can employ numerical techniques, the simplest of which is the Trapezoidal Rule. Consider the integral of $f(x)$ over the interval $[a, b]$. We begin by dividing the interval into n segments of equal length $h = \dfrac{b-a}{n}$:



Set $a = x_0$ and $b = x_n$, then the n intervals are $[x_i, x_{i+1}]$ for $i = 0 \dots n-1$.

Introductory Exercise:Trapezoidal Rule II

The area under the curve $f(x)$ now consists of integrating over each segment

$$\int_{x_i}^{x_{i+1}} f(x)\,dx$$

and summing. For each segment, we approximate the integral with the area of a trapezoid of left height $f(x_i)$ and right height $f(x_{i+1})$, giving an approximate area:

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx \frac{1}{2}h\left(f(x_i) + f(x_{i+1})\right)$$

Introductory Exercise:Trapezoidal Rule III

To see a simple case, we let $n = 3$, so $a = x_0$ and $b = x_3$, and we have

$$\frac{1}{2}h\left(f(x_0) + f(x_1)\right) + \frac{1}{2}h\left(f(x_1) + f(x_2)\right) + \frac{1}{2}h\left(f(x_2) + f(x_3)\right)$$

which can be tidied up as

$$\frac{1}{2}h\left(f(x_0) + 2f(x_1) + 2f(x_2) + f(x_3)\right)$$

so in the general case we can write

$$\int_a^b f(x)dx \approx \left(\frac{b-a}{2n}\right)\left[f(x_0) + 2\left(\sum_{i=1}^{n-1} f(x_i)\right) + f(x_n)\right]$$

Exercise I

1.) Use the Trapezoidal Rule to obtain $\mathcal{I} = \int_0^1 e^x \, dx = e - 1 \approx 1.718281828\ldots$. Let $\mathcal{I}_n$ be the approximate solution with n segments; begin by obtaining $\mathcal{I}_4$. Increase n to improve precision. Let ϵ_n be the error made with segment length $h = (b-a)/n$. For each n, calculate $\epsilon_n = |\mathcal{I} - \mathcal{I}_n|$.

2.) Tabulate your results and compare n and the error ϵ_n. Can you deduce any relationship between the error and the number of segments?

3.) Write a simple Matlab code to investigate this further. (i) Given a function $f(x)$, an interval $[a, b]$ and a number of segments n, your code should integrate the function numerically over $[a, b]$ with the interval divided into n segments. Compare with the exact solution. (ii) Next, incorporate the code you've written into a loop so you can investigate the effect of increasing n on the error. Integrate for $n = 2 \ldots N$ where N is chosen to be suitably large. Plot the error against n. What can you conclude? Hint: try a log-log plot for ϵ_n and h. Test this on several functions and intervals.

Exercise II

Now consider Simpson's rule which is a refinement of the trapezoidal rule. Take n an even number and proceed as follows:

$$\int_a^b f(x)dx \approx \left(\frac{b-a}{3n}\right)\left[f(x_0) + 2\left(\sum_{i=1}^{n/2-1} f(x_{2i})\right) + 4\left(\sum_{i=1}^{n/2} f(x_{2i-1})\right) + f(x_n)\right]$$

To see what is going on, let $n = 6$, then we have

$$\frac{h}{3}\left[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + 4f(x_5) + f(x_6)\right].$$

Repeat the previous exercise and error analysis with Simpson's rule. What do you observe?
For further reading, google "numerical integration": the wikipedia entry is well-explained and there are, as usual, many more.

Or be daring: go to the Library, find a text on Numerical Methods or Numerical Analysis (there are dozens) and look for Numerical Integration.

ODEs

An ordinary differential equation (ODE) of the form

$$y' = f(x, y)$$

may have an analytical (exact) solution. For example,

$$y' = x + y\,,$$

with initial condition $y(0) = 2$, is linear. Use integrating factor e^{-x} to find the solution

$$y = 3e^{x} - x - 1\,.$$

But more complicated functions $f(x, y)$ make this difficult or impossible. Numerical Methods are necessary.

Higher order equations

The methods used for first-order equations apply to higher order equations as well. Can always rewrite as systems of first-order equations. In the second-order equation

$$y'' = f(x, y, y')\,,$$

let $z = y'$, thus obtaining a system of coupled first-order equations:

$$z' = f(x, y, y')\,, \qquad y' = z\,.$$

For example

$$y'' - 2y' + 3y = \sin x$$

becomes

$$y' = z\,, \quad z' = 2z - 3y + \sin x\,.$$

Circuit example

The simplest LR-circuit is governed by the ODE: $L\frac{di}{dt} + Ri = V$.
(inductance L, resistance R, current i, voltage source V)
With a capacitor we have a simple LCR-circuit with a 2nd−order ODE

$$L\frac{di}{dt} + Ri + \frac{1}{C}\int i\,dt = V \Rightarrow L\frac{d^2i}{dt^2} + R\frac{di}{dt} + \frac{1}{C}i = \frac{dV}{dt}\,.$$

(capacitance C)
All of these can be solved numerically using the methods to follow.

Euler's Method I

The simplest is Euler's method. Recalling that y' is the slope of a function, we use it to calculate the slope at a point x_i and then estimate the value at a nearby point. Let (x_0, y_0) be the known initial condition. Then for a nearby point (x_1, y_1)

$$y_1 = y_0 + \left.\frac{dy}{dx}\right|_{x=x_0} (x_1 - x_0)$$

is a *linear* approximation. The smaller $h = x_1 - x_0$, the better the approximation. If we need to know some specific value $y(x_f)$, or the behaviour of the function on the interval $[x_0, x_f]$ we divide the interval into N subintervals of size h and calculate

$$y_{i+1} = y_i + \left.\frac{dy}{dx}\right|_{x=x_i} (x_{i+1} - x_i) = y_i + h\,f(x_i, y_i)\,,$$

where $N = i + 1$ completes the solution.

Euler's Method II

Example

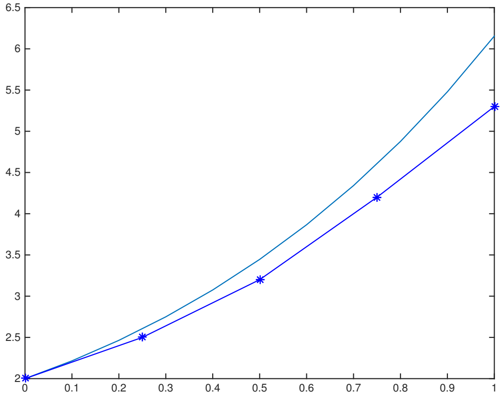
For the previous example, we have $y' = x + y$ so

$$y_{i+1} = y_i + h(x_i + y_i)$$

where $(x_0, y_0) = (0, 2)$. If we would like to obtain the behaviour of y on [0, 1], we set $x_f = 1$. Subdivide the interval into four equal pieces of length $h = 1/4$. Then

$$\begin{aligned}
y_1 &= y_0 + h(x_0 + y_0) = 2 + \frac{1}{4}(0 + 2) = 2.5 \\
y_2 &= y_1 + h(x_1 + y_1) = 2.5 + \frac{1}{4}(0.25 + 2.5) = \frac{51}{16} \approx 3.2 \\
y_3 &= y_2 + h(x_2 + y_2) = 51/16 + \frac{1}{4}(0.5 + 51/16) = \frac{263}{64} \approx 4.2 \\
y_4 &= y_3 + h(x_3 + y_3) = 263/64 + \frac{1}{4}(0.75 + 263/64) = \frac{1363}{256} \approx 5.3
\end{aligned}$$

Euler's Method III



blue: numerical solution
green: exact solution

Error I

Recall the Taylor series of a function $g(x)$ around $x = a$:

$$g(x) = g(a) + g'(a)(x-a) + \frac{g''(a)}{2}(x-a)^2 + \cdots$$

First exchange x and a:

$$g(a) = g(x) + g'(x)(a-x) + \frac{g''(x)}{2}(a-x)^2 + \cdots$$

Now let $a = x + h$, so that $a - x = h$ and we have

$$g(x+h) = g(x) + g'(x)h + \frac{g''(x)}{2}h^2 + \cdots$$

We can use this last expression to write $y(x)$ as a Taylor series around h:

$$y(x+h) = y(x) + hy'(x) + h^2\frac{y''(x)}{2} + \ldots$$

Error II

In the notation used in our implementation of Euler's method, we take $y(x_{i+1}) = y(x_i + h)$ and recall $y' = f(x, y)$, so that

$$y_{i+1} = y_i + hf(x_i, y_i) + \frac{h^2}{2} f'(x_i, y_i) + \cdots$$

so the error at each step is proportional to h^2:

$$\frac{h^2}{2} f'(x, y) = O(h^2)$$

this is called the *local* truncation error, incurred in a single iteration, from x_i to x_{i+1}. As we move from x_0 to x_f some of these errors may cancel each other out, as in some cases they may be above, in some cases below the true value of y, but this can not be relied on. In the worst case, all errors will be of the same sign, giving an estimate of the *global* truncation error as proportional to Nh^2 and since $h = \dfrac{x_f - x_0}{N}$ we see that the global error is $O(h)$.

Matlab code to evaluate Euler's method:

```
x=0; % set initial value of x0
y=2; % set yinitial condition y at x0
h=0.03; %set step-size
xf=1; %set final value of x
N=round((xf-x)/h); %nr of steps:  (interval size)/(step
size)
plot(x,y,'*'); %plot initial condition
hold on; %figure open for more data
for i=1:N %loop for N steps
y=y + h*(x+y); %next value of y
x=x+h; %increase x by stepsize
plot(x,y, 'b*') %plot now values of x,y
end
xx=0:h:xf; %same interval, stepsize
yy=3*exp(xx)-xx-1; %calculate exact solution
plot(xx,yy,'b'); %plot exact solution
```

Predictor-Corrector Methods I

An improvement on Euler's method is Heun's method, also called the "Improved Euler Method".
In Euler's method, the gradient at the beginning of an interval $[x_i, x_{i+1}]$:

$$y_i' = f(x_i, y_i)$$

is used to make a prediction of the value of y_{i+1} at the end of the interval:

$$y_{i+1}^p = y_i + hf(x_i, y_i)\,.$$

We use the superscript p to indicate the prediction and set this as the first-step of a *predictor-corrector* method, where we now estimate the gradient at the end of the interval as

$$y_{i+1}' = f(x_{i+1}, y_{i+1}^p)\,.$$

Predictor-Corrector Methods II

We now have two estimates of the gradient, one at each end of the interval, so we can estimate a better over-all gradient on $[x_i, x_{i+1}]$ as the average of the two:

$$y'_{av} = \frac{y'_i + y'_{i+1}}{2} = \frac{f(x_i, y_i) + f(x_{i+1}, y^p_{i+1})}{2}\,.$$

Predictor-Corrector Methods III

Using this average gradient, we can now use Euler's method to estimate y_{i+1}:

$$y_{i+1} = y_i + h\left(\frac{y_i' + y_{i+1}'}{2}\right) = y_i + h\left(\frac{f(x_i, y_i) + f(x_{i+1}, y_{i+1}^p)}{2}\right),$$

which is called the *corrector* equation.
The method is summed up as

$$\begin{array}{rcll} y_{i+1}^p &=& y_i + hf(x_i, y_i) & \text{Predictor equation} \\ y_{i+1} &=& y_i + h\left(\frac{f(x_i,y_i)+f(x_{i+1},y_{i+1}^p)}{2}\right) & \text{Corrector equation} \end{array}$$

Note that the corrector equation includes two distinct values of the unknown $y(x_{i+1})$, the first estimate y_{i+1}^p and the second y_{i+1}. This can be seen as an iteration: use the corrector equation repeatedly to improve the estimate of y_{i+1}. This will not necessarily converge on the exact value of y but can significantly reduce the local truncation error.

Second-order Runge-Kutta I

Runge-Kutta methods have several orders, there is one of order 1: the Euler method, but there are infinitely many of order 2, of which we have seen only two.
In general, we write

$$y_{i+1} = y_i + h\phi(x_i, y_i, h)$$

where ϕ is called the *increment* function and can be interpreted as an optimal representation of the gradient of y over the interval $[x_i, x_{i+1}]$. The increment function can be written as

$$\phi = a_1k_1 + a_2k_2 + \dots a_nk_n$$

Second-order Runge-Kutta II

where the a_i are constants and the k_i are

$$
\begin{aligned}
k_1 &= f(x_i\,, y_i) \\
k_2 &= f(x_i + p_1 h\,, y_i + q_{11} k_1 h) \\
k_3 &= f(x_i + p_2 h\,, y_i + q_{21} k_1 h + q_{22} k_2 h) \\
&\cdot \\
&\cdot \\
&\cdot \\
k_n &= f(x_i + p_{n-1} h, y_i + q_{n-1,1} k_1 h + q_{n-1,2} k + 2h + \ldots + q_{n-1,n-1} k_{n-1} h)
\end{aligned}
$$

for an n^{th} order RK method. The k_i are obtained recurrently, easy to implement in any programming environment. For $n = 1$ there is only one term k_1, giving Euler's method. For $n = 2$ we require constants p_1 and q_{11} and weights a_1, a_2. Using Taylor expansion we can obtain three equations for these, so they are not uniquely determined: there are infinitely many second-order RK methods.

Derivation of Second-order RK I

We have $y_{i+1} = y_i + h(ak_1 + bk_2)$, where $k_1 = f(x_i\,, y_i)$, and $k_2 = f(x_i + ph\,, y_i + qk_1 h)$, where we drop indices for optical simplicity and seek a, b, p, q. We begin with the Taylor expansion we saw earlier:

$y(x+h) = y(x) + hy'(x) + \frac{h^2}{2!}y''(x) + ...$ giving

$y_{i+1} = y_i + hf(x_i, y_i) + \frac{h^2}{2}f'(x_i, y_i) + \cdots$. where we use partial differentiation to obtain $f'(x,y) = \frac{\partial f(x,y)}{\partial x} + \frac{\partial f(x,y)}{\partial y}\frac{dy}{dx}$, so that

$$y_{i+1} = y_i + hf(x_i, y_i) + \frac{h^2}{2}\left(\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{dy}{dx}\right) + \dots \qquad (**)$$

Derivation of Second-order RK II

Now consider $k_2 = f(x_i + ph\,, y_i + qk_1h)$. Recall the Taylor expansion for a function of two variables:

$$F(x+h, y+k) = F(x,y) + h\frac{\partial F}{\partial x} + k\frac{\partial F}{\partial y} + O(h^2, k^2)$$

which we apply to obtain

$$k_2 = f(x_i + ph\,, y_i + qk_1h) = f(x_i, y_i) + ph\frac{\partial f}{\partial x} + qk_1h\frac{\partial f}{\partial y} + O(h^2)\,.$$

Substituting for k_1 and k_2 into $y_{i+1} = y_i + h(ak_1 + bk_2)$ we have

$$\begin{aligned} y_{i+1} &= y_i + hak_1 + hbk_2 \\ &= y_i + haf(x_i\,, y_i) + hb\left[f(x_i, y_i) + ph\frac{\partial f}{\partial x} + qf(x_i\,, y_i)h\frac{\partial f}{\partial y} + O(h^2)\right] \\ &\qquad \text{and collect terms:} \\ &= y_i + (a+b)hf(x_i, y_i) + h^2\left(bp\frac{\partial f}{\partial x} + bq\frac{\partial f}{\partial y}f(x_i\,, y_i)\right) + O(h^3) \end{aligned}$$

Derivation of Second-order RK III

Now compare this last equation with $(**)$, not forgetting that $dy/dx = f(x_i, y_i)$, to see that we require

$$\begin{aligned} a+b &= 1 \\ bp &= 1/2 \\ bq &= 1/2 \end{aligned}$$

which is a system of 3 equations in 4 unknowns, with infinitely many solutions.
Choose for example $b = 1/2$, so that $a = 1/2$ and $p = q = 1$. This gives

$$y_{i+1} = y_i + h\left(\frac{1}{2}k_1 + \frac{1}{2}k_2\right)$$

where $k_1 = f(x_i\,, y_i)$, and $k_2 = f(x_i + h\,, y_i + k_1 h)$. Noting that k_1, resp. k_2, is the gradient at the beginning, resp. end of the interval, this is just the Heun method with a single correction y^p_{i+1}.

Derivation of Second-order RK IV

Each choice of b gives a new variation, each with the same rough global error $O(h^2)$ but differences in finer detail, see any text on Numerical Analysis for more detail.

Midpoint method I

Another, similar, approach improves Euler's method, based on using Euler's method to estimate the gradient at the midpoint of the interval $[x_i, x_{i+1}]$ and using this to obtain a better estimate of y at the endpoint.
In terms of the RK2 notation used above, we let $b = 1$, so that $a = 0$ and $p = q = 1/2$ giving

$$y_{i+1} = y_i + hk_2$$

where k_1 is as usual, and $k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right)$, which is the midpoint method.

$$\begin{aligned} k_1 &= f(x_i, y_i) && \text{gradient at } x_i \text{ using Euler} \\ k_2 &= f(x_i + 0.5h, y_i + 0.5hk_1) && \text{gradient at } x_i + h/2 \text{ using Euler} \\ y_{i+1} &= y_i + hk_2 \end{aligned}$$

Higher-order Runge-Kutta Methods

There are many, here is just one of the most common in use, the:

Classic fourth order Runge-Kutta method

$$\begin{aligned} k_1 &= f(x_i\,, y_i) \\ k_2 &= f(x_i + 0.5h\,, y_i + 0.5k_1 h) \\ k_3 &= f(x_i + 0.5h\,, y_i + 0.5k_2 h) \\ k_4 &= f(x_i + h\,, y_i + k_3 h) \end{aligned}$$

combined with

$$y_{i+1} = y_i + h\left(\frac{1}{6}k_1 + \frac{1}{3}k_2 + \frac{1}{3}k_3 + \frac{1}{6}k_4\right)$$

Error Analysis I

If the ODE is of the form $y' = f(x)$, a function of x only, the predictor step is not required, as we can obtain the average gradient directly from x_i and x_{i+1} so that a single application of the corrector step gives

$$y_{i+1} = y_i + h\left(\frac{f(x_i) + f(x_{i+1})}{2}\right), \qquad (*)$$

which looks remarkably like the trapezoidal method of numerical integration. Let's explore this. We can solve the ODE $y' = f(x)$ by integrating over the appropriate interval:

$$\int_{y_i}^{y_{i+1}} dy = \int_{x_i}^{x_{i+1}} f(x)\,dx \Rightarrow y_{i+1} - y_i = \int_{x_i}^{x_{i+1}} f(x)\,dx\,.$$

Error Analysis II

Recall that the trapezoidal method approximates

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx h\left(\frac{f(x_i)+f(x_{i+1})}{2}\right)$$

where $h = x_{i+1} - x_i$. Hence the error in $(*)$ is given by the error in the Trapezoidal method: a heuristic error analysis of this method gave the global truncation error as $O(h^2)$, and the same applies to Heun's method, though we do not show this analytically. It can be shown that for the general case $y' = f(x,y)$, the same error holds.

Higher order ODE - Coupled first order ODEs I

A second order, or higher system, can be written as a system of first-order equations:

$$\frac{d^2x}{dt^2} + 2\frac{dx}{dt} - 3x = \sin t$$

with initial conditions $x(0) = x'(0) = 0$. Taking $y = x'$ we have $y' = x''$ giving the system of two coupled first-order ODEs:

$$x' = y = f_1(t, x, y) , \quad y' = \sin t + 3x - 2y = f_2(t, x, y) ,$$

with initial conditions $x(0) = y(0) = 0$, which can be solved by any of the RK methods. Though f_1 is not actually a function of t, x, we write it with all three arguments, for the case of where we have two coupled first-order equations which can be functions of all three variables. The method can be generalized in an obvious way for an ODE of order n giving n coupled first-order ODEs.

Higher order ODE - Coupled first order ODEs II

We illustrate by employing Euler's and Heun's method to solve the system. Note that where we had one dependent variable y and one independent variable x, we now have two dependent variables x, y and one independent variable t. So we will have increments in time: $t_{i+1} = t_i + h$ giving increments in x and y:

$$\begin{aligned} x_{i+1} &= x_i + h\,\phi_x(t_i, x_i, y_i) \\ y_{i+1} &= y_i + h\,\phi_y(x_i, y_i, y_i) \end{aligned}$$

The increments for Euler and second-order RK are given as

$$\begin{aligned} \phi_x &= ak_{1x} + bk_{2x} \\ \phi_y &= ak_{1y} + bk_{2y}\,, \end{aligned}$$

where $a = 1, b = 0$ for Euler's method and $a = b = 1/2$ for Heun's method.

Higher order ODE - Coupled first order ODEs III

For Euler's method, the easiest case, we have

$$\begin{aligned} k_{1x} = \quad & f_1(t_i, x_i, y_i) \quad && = y_i \\ k_{1y} = \quad & f_2(t_i, x_i, y_i) \quad && = \sin t_i + 3x_i - 2y_i \end{aligned}$$

which means we can skip the $\phi = ak_1$ stage and write

$$\begin{aligned} x_{i+1} &= x_i + h\, y_i \\ y_{i+1} &= y_i + h(\sin t_i + 3x_i - 2y_i) \end{aligned}$$

with the usual $x_0 = 0$ and $y_0 = 0$, for $t_0 = 0$. We divide up the interval, say [0, 1] into n equal segments of length $h = 1/n$ and iterate as before, calculating two new values, x_{i+1} and y_{i+1} at each stage, increasing t_i by h until $t_n = 1$. To see this in action, let $h = 0.2$, and begin Euler's iteration:

Higher order ODE - Coupled first order ODEs IV

$$\begin{aligned} x_1 &= x_0 + h\,y_0 = 0 + 0.2(0) = 0 \\ y_1 &= y_0 + h(\sin t_0 + 3x_0 - 2y_0) = 0 \end{aligned}$$

which looks odd, but keep on iterating. Increase t to $t_1 = 0.2$, then

$$\begin{aligned} x_2 &= x_1 + h\,y_1 &&= 0 + 0.2(0) = 0 \\ y_2 &= y_1 + h(\sin t_1 + 3x_1 - 2y_1) &&= 0 + 0.2(\sin 0.2 + 0 - 0) \approx 0.03973 \end{aligned}$$

and increase t to $t_2 = 0.4$:

$$\begin{aligned} x_3 &= x_2 + h\,y_2 &&\approx 0 + 0.2(0.03973) \approx 0.007947 \\ y_3 &= y_2 + h(\sin t_2 + 3x_2 - 2y_2) &&\approx 0.03973 + 0.2(\sin 0.4 + 0 - 2(0.03973)) \\ & &&\approx 0.1017 \end{aligned}$$

Higher order ODE - Coupled first order ODEs V

and so on. Doing this with increasing order of RK method just requires care. We illustrate it with Heun's method. Here we have

$$\begin{aligned} k_{1x} = &\ f_1(t_i, x_i, y_i) &= y_i \\ k_{1y} = &\ f_2(t_i, x_i, y_i) &= \sin t_i + 3x_i - 2y_i \end{aligned}$$

as before, and

$$\begin{aligned} k_{2x} &= f_1(t_i + ph, x_i + hqk_{1x}, y_i + hqk_{1y}) \\ &= y_i + hk_{1y} \\ k_{2y} &= f_2(t_i + ph, x_i + hqk_{1x}, y_i + hqk_{1y}) \\ &= \sin(t_i + h) + 3(x_i + hk_{1x}) - 2(y_i + hk_{1y}) \end{aligned}$$

(recall that for Heun $p = q = 1$) giving the increments, and so

$$\begin{aligned} x_{i+1} &= x_i + h(ak_{1x} + bk_{2x}) = x_i + \tfrac{h}{2}(k_{1x} + k_{2x}) \\ y_{i+1} &= y_i + h(ak_{1y} + bk_{2y}) = y_i + \tfrac{h}{2}(k_{1y} + k_{2y}) \end{aligned}$$

as $a = b = 1/2$ for Heun.

Finite Differences for ODE I

Finite Difference methods take a different approach to those seen up to now. For a second-order, or higher, ODE, we can distinguish between an IVP, where all the information is known at the same (initial) point and a Boundary Value Problem, BVP where, for example
$y'' - 2y' + 3y = \sin x$, with $y(0) = 0$ and $y(1) = 0$. We have two conditions on y, needed to specify a second-order system but now we have information on y at two different points, usually thought of as the boundaries of an interval of interest. We may similarly have $y'(0) = -1$, $y'(1) = 1$ or other variations.
Note: Unlike IVPs, solutions to BVPs do not necessarily exist, see any text on Differential equations, for example "Elementary Differential Equations and Boundary value problems" by Boyce/Di Prima. We will not concern ourselves with this problem and deal only with BVPs where solutions exist.

Finite Differences for ODE II

The approach followed previously will not work here. If we represent the second-order equation as a system of two first-order equations in y and $z = y'$, the boundary conditions $y(0) = 0$ and $y(1) = 0$ do not tell us anything about z so we have no z_0 to start off the process. Worse, even if we did, we can start off the process at y_0 but cannot guarantee in any sensible way that the iteration would lead to $y_n = y(1)$ as given. Similar problems arise for other possible combinations of the boundary conditions. What is to be done? A burning question!

Finite Differences for ODE III

One solution (among several) lies in breaking up the interval in question, in this case $[0, 1]$. We begin by finding an approximation for the second derivative. Define the *central difference*

$$\delta y(x_i) = y\left(x_i + \frac{h}{2}\right) - y\left(x_i - \frac{h}{2}\right) ,$$

and note that

$$\frac{1}{h}\delta y(x_i) = \frac{y(x_i + \frac{h}{2}) - y(x_i - \frac{h}{2})}{h} \approx \left.\frac{dy}{dx}\right|_{x=x_i}$$

Finite Differences for ODE IV

Similarly, the second central difference is $\delta^2 y(x_i) =$

$$\begin{aligned}
&= \delta(\delta y(x_i)) \\
&= \delta y\left(x_i + \frac{h}{2}\right) - \delta y\left(x_i - \frac{h}{2}\right) \\
&= y\left[\left(x_i + \frac{h}{2}\right) + \frac{h}{2}\right] - y\left[\left(x_i + \frac{h}{2}\right) - \frac{h}{2}\right] \\
&\qquad - \left\{ y\left[\left(x_i - \frac{h}{2}\right) + \frac{h}{2}\right] - y\left[\left(x_i - \frac{h}{2}\right) - \frac{h}{2}\right] \right\} \\
&= y(x_i + h) - 2y(x_i) + y(x_i - h)
\end{aligned}$$

Since the second derivative y'' is the first derivative of y', a similar argument gives

$$\frac{1}{h^2}\delta^2 y(x_i) \approx \left.\frac{d^2y}{dx^2}\right|_{x=x_i}$$

Finite Differences for ODE V

To approximate the first derivative in terms of $x_i \pm h$, we proceed slightly differently. Take the central difference this time with $\Delta y(x_i) = y(x_i + h) - y(x_i - h)$ so that

$$\frac{1}{2h}\Delta y(x_i) = \frac{y(x_i + h) - y(x_i - h)}{2h} = \frac{y(x_{i+1}) - y(x_{i-1})}{2h} \approx \left.\frac{dy}{dx}\right|_{x=x_i}$$

We now take $u_i \approx y(x_i)$ so we can approximate

$$\left.\frac{dy}{dx}\right|_{x=x_i} \approx \frac{u_{i+1} - u_{i-1}}{2h}, \quad \text{and} \quad \left.\frac{d^2y}{dx^2}\right|_{x=x_i} \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}.$$

Example I

We take the model convection-diffusion equation

$$y'' - 20y' = -1\,, \quad \text{with } y(0) = 1\,, y(1) = 0\,.$$

We divide the interval of interest $[0, 1]$ into five equal segments of length $h = 1/5$, giving $x_0 = 0\,, x_1 = 0.2\,, x_2 = 0.4\,, x_3 = 0.6\,, x_4 = 0.8\,, x_5 = 1$. Estimating the derivatives using the formulae in the previous slide, we get

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} - 20\left(\frac{u_{i+1} - u_{i-1}}{2h}\right) = -1$$

and rearrange to

Example II

$$\left(\frac{10}{h}+\frac{1}{h^2}\right)u_{i-1}-\frac{2}{h^2}u_i+\left(-\frac{10}{h}+\frac{1}{h^2}\right)u_{i+1}=-1$$

or simply

$$au_{i-1}+bu_i+cu_{i+1}=-1\,,$$

where
$a=10/h+1/h^2=75\,,\,b=-2/h^2=-50$ and $c=-10/h+1/h^2=-25$

for $i=1,2,3,4$, and $u_0=1\,,u_5=0$.

Example III

Each $i = 1..4$ is an equation involving u_{i-1}, u_i, u_{i+1} :

$$\begin{array}{cccccccc}
au_0+ & bu_1+ & cu_2 & & & & = -1 \\
 & au_1+ & bu_2+ & cu_3 & & & = -1 \\
 & & au_2+ & bu_3+ & cu_4 & & = -1 \\
 & & & au_3+ & bu_4+ & cu_5 & = -1
\end{array}$$

As we know u_0 and u_5 the first and last equations involve only two unknowns, and we can rewrite in matrix form

$$\begin{pmatrix} b & c & 0 & 0 \\ a & b & c & 0 \\ 0 & a & b & c \\ 0 & 0 & a & b \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = \begin{pmatrix} -1 - au_0 \\ -1 \\ -1 \\ -1 - cu_5 \end{pmatrix}$$

Example IV

The solution is easily obtained with Gaussian elimination. In this case, $u_1 \approx 0.9928\,, u_2 \approx 1.0544\,, u_3 \approx 0.9095\,, u_4 \approx 1.3843\,.$
A matrix of this type is called "tridiagonal". The solution of larger matrices is best done using numerical algorithms, of which many exist.

Finite Differences for PDEs: Heat/Diffusion Equation I

The method of finite differences extends nicely to the solution of Partial Differential Equations. Again, many solution methods exist, for many types of PDEs. Here we take a brief look at one method and two simple types of PDE.

1. Heat or Diffusion equation

$$\frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial x^2}\,, \quad 0 < x < 1\,, \quad t > 0$$

with Boundary Conditions $y(0,t) = y(1,t) = 0$ and initial condition $y(x,0) = y_0(x)$ describes the temperature distribution in a thin metal rod of length 1, with insulated sides and both ends kept at temperature zero. At time $t = 0$, the distribution is $y_0(x)$ and the solution of the PDE describes the evolution in time. The PDE can also be used to describe other diffusive processes, for example, pollutant gas in a pipe, or a random walk.

Finite Differences for PDEs: Heat/Diffusion Equation II

The novelty here is that we will employ finite differences for both derivatives.
We begin by dividing the spatial interval into N segments of equal length $h = 1/N$:
$x_0 = 0, x_1 = h, x_2 = 2h, \ldots, x_N = Nh = 1\,.$
We do the same in the time domain, discretize time into equal segments of length k:
$t_0 = 0, t_1 = k, t_2 = 2k, \ldots$
Note there is no clear end: we iterate the process as far as we need to get to some value t_f, but it is best to look at the value of y for several carefully chosen values of t to see the evolution in time.
We let U_j^m be the value $y(x_j, t_m)$. The initial condition gives the values of y at time $t = 0$:
$U_j^0 = y(x_j, t_0) = y(x_j, 0) = y_0(x_j)\,.$ for $j = 0, 1, 2, \ldots N$.
The initial condition gives all U_j^0. The Boundary condition gives the values for $j = 0$, corresponding to $x = 0$, and for $j = N$, where $x = 1$:
$U_j^m = y(x_j, t_m) \Rightarrow y(0, t_m) = U_0^m = 0\,,$ and $y(1, t_m) = U_N^m = 0\,, \forall m \geq 0\,.$

Finite Differences for PDEs: Heat/Diffusion Equation III

For the spatial derivative, we use the previously obtained central difference, with a slight change in notation, as we now have a function of two variables. So

$$\frac{\partial^2 y(x,t)}{\partial x^2} \approx \frac{y(x+h,t) - 2y(x,t) + y(x-h,t)}{h^2}$$

where only x varies by h in both directions, and t stays constant. So when $x = x_j$ and $t = t_m$, we have $x \pm h = x_{j\pm 1}$:

$$\begin{aligned} \frac{\partial^2 y(x_j, t_m)}{\partial x^2} &\approx \frac{y(x_{j+1}, t_m) - 2y(x_j, t_m) + y(x_{j-1}, t_m)}{h^2} \\ &= \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{h^2}, \qquad j = 1, 2, \ldots N-1 \end{aligned}$$

Finite Differences for PDEs: Heat/Diffusion Equation IV

For the time derivative, we use a new "forward difference". We estimate

$$\frac{\partial y(x,t)}{\partial t} \approx \frac{y(x,t+k)-y(x,t)}{k}$$

This is necessary as we don't have any information for a time $t=-1$, so using a centred difference here makes no sense. Note the similarity to Euler's method for ODEs. Again, when $x = x_j$ and $t = t_m$, we have $t + k = t_{m+1}$, so that:

$$\begin{aligned}\frac{\partial y(x_j,t_m)}{\partial t} &\approx \frac{y(x_j,t_{m+1})-y(x_j,t_m)}{k}\\ &= \frac{U_j^{m+1}-U_j^m}{k}, \qquad m = 0,1,2,3\dots\end{aligned}$$

Finite Differences for PDEs: Heat/Diffusion Equation V

Finally, set the two derivatives equal and we have

$$\frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{h^2} = \frac{U_j^{m+1} - U_j^m}{k}$$

Let $k/h^2 = v$ and rearrange to

$$v\left(U_{j+1}^m - 2U_j^m + U_{j-1}^m\right) = U_j^{m+1} - U_j^m$$

Note that there is only one term at time t_{m+1}, and many at time t_m. This gives the algorithm: knowing U_j^0, for all j, from the initial condition, we can find U_j^1 from these using the last equation rearranged as:

$$U_j^{m+1} = U_j^m + v\left(U_{j+1}^m - 2U_j^m + U_{j-1}^m\right) = vU_{j-1}^m + (1-2v)U_j^m + vU_{j+1}^m$$

Finite Differences for PDEs: Heat/Diffusion Equation VI

It will be easier to see what is going on with an example. Let $N = 5$, then $j = 1..4$ gives the required set of five equations:

$$\begin{array}{lllllll} U_1^{m+1} & = & vU_0^m & +\beta U_1^m & +vU_2^m & & \\ U_2^{m+1} & = & & vU_1^m & +\beta U_2^m & +vU_3^m & \\ U_3^{m+1} & = & & & vU_2^m & +\beta U_3^m & +vU_4^m \\ U_4^{m+1} & = & & & & vU_3^m \quad +\beta U_4^m & +vU_5^m \end{array}$$

(with $\beta = 1 - 2v$.) There is no need to calculate U_0^{m+1} or U_5^{m+1}: these are the boundary values, both equal to zero, for all m. Note that the above gives an algorithm. Given at time $t = 0 \Rightarrow m = 0$, with initial values U_j^0 for $j = 0...5$, we use

$$U_j^1 = vU_{j-1}^0 + (1 - 2v)U_j^0 + vU_{j+1}^0 ,$$

and each U_j^1 is calculated from three values U_j^0, the three neighbours, centred on U_j^0, so that

Finite Differences for PDEs: Heat/Diffusion Equation VII

$$\begin{array}{lllllll} U_1^1 & = & vU_0^0 & +\beta U_1^m & +vU_2^0 & & \\ U_2^1 & = & & vU_1^0 & +\beta U_2^0 & +vU_3^0 & \\ U_3^1 & = & & & vU_2^0 & +\beta U_3^0 & +vU_4^0 \\ U_4^1 & = & & & & vU_3^0 & +\beta U_4^0 \quad +vU_5^0 \end{array}$$

and so on, iterating over m and at each stage obtaining U_j^{m+1} from three values of U_j^m. Here we have zero boundary conditions, so that $U_0^m = U_5^m = 0, \forall m \geq 0$, but it should be clear that non-zero constant boundary conditions, or even boundary conditions that vary with time would not present much additional difficulty to implement in this algorithm. Error analysis shows that we require $v \leq 1/2$ for stability.

Laplace/Poisson Equation I

Poisson's equation for 2 variables in the plane is $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = g(x, y)$, which gives Laplace's equation when $g = 0$.
The key here is that we will use the central difference to approximate both derivatives. We have seen how the central difference works. We discretize the spatial domain into segments of length h in both directions, so that

$$
\begin{aligned}
\frac{\partial^2 u(x,y)}{\partial x^2} &\approx \frac{u(x+h,y) - 2u(x,y) + u(x-h,y)}{h^2} \\
\frac{\partial^2 u(x_i,y_j)}{\partial x^2} &\approx \frac{u(x_{i+1},y_j) - 2u(x_i,y_j) + u(x_{i-1},y_j)}{h^2} = \frac{U^j_{i+1} - 2U^j_i + U^j_{i-1}}{h^2},
\end{aligned}
$$

Laplace/Poisson Equation II

and similarly

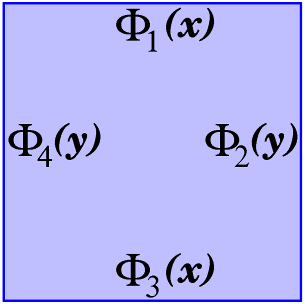
$$
\begin{aligned}
\frac{\partial^2 u(x,y)}{\partial y^2} &\approx \frac{u(x,y+h) - 2u(x,y) + u(x,y-h)}{h^2} \\
\frac{\partial^2 u(x_i,y_j)}{\partial y^2} &\approx \frac{u(x_i,y_{j+1}) - 2u(x_i,y_j) + u(x_i,y_{j-1})}{h^2} = \frac{U_i^{j+1} - 2U_i^j + U_i^{j-1}}{h^2}.
\end{aligned}
$$

Set the sum of the two equal to zero gives the approximation for Laplace's equation:

$$
\begin{aligned}
\frac{U_{i+1}^j - 2U_i^j + U_{i-1}^j}{h^2} \quad + \quad & \frac{U_i^{j+1} - 2U_i^j + U_i^{j-1}}{h^2} = 0 \\
& \Rightarrow U_{i+1}^j + U_{i-1}^j + U_i^{j+1} + U_i^{j-1} - 4U_i^j = 0
\end{aligned}
$$

Laplace/Poisson Equation III

The simplest case of Laplace's equations is on a rectangle, taken as $0 \leq x \leq a$ and $0 \leq y \leq b$ which is divided into $(n-1)x(m-1)$ squares with side length h, so that $a = nh$ and $b = mh$ and so $i = 1 \ldots n$ and $j = 1 \ldots m$. The solution requires knowledge of u on the boundaries. Let $u(x,b) = \phi_1(x)$, $u(a,y) = \phi_2(y)$, $u(x,0) = \phi_3(x)$, and $u(0,y) = \phi_4(y)$ be the given boundary conditions:



Laplace/Poisson Equation IV

Then the known functions give us values of U on the outside of the grid:
$\phi_1(x)$, where $y = b$, gives the values U_i^m, for $i = 1 \ldots n$;
$\phi_2(y)$, where $x = a$, gives the values U_n^j, for $j = 1 \ldots m$;
$\phi_3(x)$, where $y = 0$, gives the values U_i^1, for $i = 1 \ldots n$;
$\phi_4(y)$, where $x = 0$, gives the values U_1^j, for $j = 1 \ldots m$.

Laplace/Poisson Equation V

To see this, break up a square, with $a = b$, into a grid with 5×5 points, so that $i, j = 1 \ldots 5$:

$$\begin{array}{ccccccccc}
U_1^5 & -- & U_2^5 & -- & U_3^5 & -- & U_4^5 & -- & U_5^5 \\
| & & | & & | & & | & & | \\
| & & | & & | & & | & & | \\
U_1^4 & -- & P_7 & -- & P_8 & -- & P_9 & -- & U_5^4 \\
| & & | & & | & & | & & | \\
| & & | & & | & & | & & | \\
U_1^3 & -- & P_4 & -- & P_5 & -- & P_6 & -- & U_5^3 \\
| & & | & & | & & | & & | \\
| & & | & & | & & | & & | \\
U_1^2 & -- & P_1 & -- & P_2 & -- & P_3 & -- & U_5^2 \\
| & & | & & | & & | & & | \\
| & & | & & | & & | & & | \\
U_1^1 & -- & U_2^1 & -- & U_3^1 & -- & U_4^1 & -- & U_5^1
\end{array}$$

Laplace/Poisson Equation VI

The values U_i^j on the edges are known from the BCs. Only the values of the interior points $P_1 \dots P_9$ are unknown. The approximation of Laplace's equation gives us

$$U_{i+1}^j + U_{i-1}^j + U_i^{j+1} + U_i^{j-1} - 4U_i^j = 0$$

which is a relation involving five points, one at the centre, at (x_i, y_j) and one each above, below, to the right and to the left of the central point. If we apply this relation, taking every interior point P_k in turn as the centre of such a relation, we get

$$\begin{aligned}
\text{at } P_1 &: \quad U_1^2 + U_2^1 + P_2 + P_4 - 4P_1 = 0 \\
\text{at } P_2 &: \quad P_1 + U_3^1 + P_3 + P_5 - 4P_2 = 0 \\
\text{at } P_3 &: \quad P_2 + U_4^1 + U_5^2 + P_6 - 4P_3 = 0
\end{aligned}$$

Laplace/Poisson Equation VII

and so on. Obtain the remaining six equations and rewrite in matrix form:

$$\begin{pmatrix} -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 \end{pmatrix} \begin{pmatrix} P_1 \\ P_2 \\ P_3 \\ P_4 \\ P_5 \\ P_6 \\ P_7 \\ P_8 \\ P_9 \end{pmatrix}$$

$$= -\left(U_2^1 + U_1^2, U_3^1, U_4^1 + U_5^2, U_1^3, 0, U_5^3, U_1^4 + U_2^5, U_3^5, U_4^5 + U_5^4\right)^T$$

Which can be solved with matrix methods, taking advantage of the many zero entries and clear patterns.

Nevertheless, for large systems, this is computationally expensive and an alternative is the **Relaxation** method.

Laplace/Poisson Equation VIII

Relaxation method.

Begin by setting all points inside the grid to an initial value k, obtained as the average of the values of the known boundary points.
Continuity of solutions suggests that we can take each point as the average of its four nearest neighbours on the grid:

$U_i^j = (U_{i+1}^j + U_{i-1}^j + U_i^{j+1} + U_i^{j-1})/4$ so that

$$\frac{U_{i+1}^j + U_{i-1}^j + U_i^{j+1} + U_i^{j-1} - 4U_i^j}{4} = 0$$

Initially this is not the case: all interior points are set to k.

Laplace/Poisson Equation IX

Then for each interior point, we can calculate

$$\left(U_i^j\right)_{\text{new}} = \left(U_i^j\right)_{\text{old}} + r_i^j$$

where the *residual* r_{ij} is given by

$$r_i^j = \frac{U_{i+1}^j + U_{i-1}^j + U_i^{j+1} + U_i^{j-1} - 4U_i^j}{4}$$

which vanishes as the averages are recalculated repeatedly. Set a desired accuracy $\epsilon > 0$ and stop when $|r_i^j| < \epsilon$ at every interior point.
It is possible to accelerate the convergence of this process, resulting in the so-called Successive Over-Relaxation or SOR method.

Laplace/Poisson Equation X

If we're dealing with the Poisson equation instead of the Laplace equation, we have a non-zero term $g(x,y)$ on the r.h.s. in the original PDE.
By taking $g(x_i,y_j)=g_i^j$, this is easily included in any of the above schemes, for example for the relaxation method we get

$$r_i^j = \frac{U_{i+1}^j + U_{i-1}^j + U_i^{j+1} + U_i^{j-1} - 4U_i^j - h^2 g_i^j}{4} .$$

$\mathcal{THE\ END}$