Differential Equations

We will cover a few different methods to solve first-order ordinary differential equations (first-order means first derivative; ordinary means a function of only one independent variable). The problem is given by

$$\frac{dx}{dt} = f(x,t) \tag{1}$$

To find the solution $x(t)$, we need to know $f(x,t)$ and an initial condition, i.e. the value of x at some particular time t.

1 The Euler Method

Recall the general definition of the Taylor expansion; the Taylor expansion of a function $g(z)$ about the point $z = a$:

$$g(z) = \sum_{i=0}^{\infty} \frac{g^{(i)}(a)}{i!}(z-a)^i \tag{2}$$

Let $z = t + h$ and $a = t$ and let's make a Taylor expansion of the function $x(z)$ about the point $z = a$:

$$\begin{aligned}
x(z) &= \sum_{i=0}^{\infty} \frac{x^{(i)}(a)}{i!}(z-a)^i \\
x(t+h) &= \sum_{i=0}^{\infty} \frac{x^{(i)}(t)}{i!}(t+h-t)^i \\
x(t+h) &= \sum_{i=0}^{\infty} \frac{x^{(i)}(t)}{i!}(h)^i \\
x(t+h) &= x(t) + h\frac{dx}{dt} + \frac{1}{2}h^2\frac{d^2x}{dt^2} + ... \\
x(t+h) &= x(t) + hf(x,t) + \mathcal{O}(h^2) \qquad (3)
\end{aligned}$$

If h is small enough, we can neglect terms of order h^2 and higher, leaving

$$x(t+h) \approx x(t) + hf(x,t) \tag{4}$$

Given the value of $x(t)$ at some particular time (the initial condition), we can approximate the value of x a short time later ($x(t+h)$).

Let's say that $x(t_0) = x_0$. We can calculate $x(t_0 + h)$ given $x(t_0)$ using the equation above. Once we know $x(t_0 + h)$, we can use the equation above again to find $x(t_0 + 2h)$. And you can continue on to map out the function $x(t)$ at evenly spaced points, using

$$x_i(t_i) = x_{i-1} + hf(x_{i-1}, t_{i-1}) \tag{5}$$

where $t_i = t_0 + ih$ and $x_i = x(t_i)$.

To find the function value n steps away from the known value, where each step has size $\Delta t = h$:

$$\begin{aligned}
x(t+h) &= x(t) + hf(x,t) \\
x(t+2h) &= x(t+h) + hf(x(t+h), t+h) \\
&= x(t) + hf(x,t) + hf(x(t+h), t+h) \\
x(t+3h) &= x(t+2h) + hf(x(t+2h), t+2h) \\
&= x(t) + hf(x,t) + hf(x(t+h), t+h) + hf(x(t+2h), t+2h) \\
&\dots \qquad (6) \\
x(t+nh) &= x(t) + \sum_{k=1}^{n-1} hf(x(t+kh), t+kh) \qquad (7)
\end{aligned}$$

Example: Euler Method 1
Example: Euler Method 2

Section 3, Exercise 1

2 The Runge-Kutta Method

The Runge-Kutta method is really a set of methods. In fact, Euler's method is the first-order Runge-Kutta method. Let's consider the second order Runge-Kutta method (sometimes called the midpoint method).

We perform another Taylor expansion. In Equation 2, let $z = t + h$ and $a = t + h/2$ and let's make a Taylor expansion of the function $x(z)$ about the point $z = a$:

$$
\begin{aligned}
x(z) &= \sum_{i=0}^{\infty} \frac{x^{(i)}(a)}{i!}(z-a)^i \\
x(t+h) &= \sum_{i=0}^{\infty} \frac{x^{(i)}(t+h/2)}{i!}(t+h-(t+h/2))^i \\
x(t+h) &= \sum_{i=0}^{\infty} \frac{x^{(i)}(t+h/2)}{i!}\left(\frac{h}{2}\right)^i \\
x(t+h) &= x(t+h/2) + \frac{h}{2}\left.\frac{dx}{dt}\right|_{t+h/2} + \frac{1}{2}\left(\frac{h}{2}\right)^2 \left.\frac{d^2x}{dt^2}\right|_{t+h/2} + ... \qquad (8)
\end{aligned}
$$

We do it again, letting $z = t$ and $a = t + h/2$:

$$
\begin{aligned}
x(z) &= \sum_{i=0}^{\infty} \frac{x^{(i)}(a)}{i!}(z-a)^i \\
x(t) &= \sum_{i=0}^{\infty} \frac{x^{(i)}(t+h/2)}{i!}(t-(t+h/2))^i \\
x(t) &= \sum_{i=0}^{\infty} \frac{x^{(i)}(t+h/2)}{i!}\left(-\frac{h}{2}\right)^i \\
x(t) &= x(t+h/2) - \frac{h}{2}\left.\frac{dx}{dt}\right|_{t+h/2} + \frac{1}{2}\left(\frac{h}{2}\right)^2 \left.\frac{d^2x}{dt^2}\right|_{t+h/2} - ... \qquad (9)
\end{aligned}
$$

Subtract the second expression from the first:

$$
\begin{aligned}
x(t+h) - x(t) &= x(t+h/2) + \frac{h}{2}\left.\frac{dx}{dt}\right|_{t+h/2} + \frac{1}{2}\left(\frac{h}{2}\right)^2 \left.\frac{d^2x}{dt^2}\right|_{t+h/2} + ... \\
&\quad - \left[x(t+h/2) - \frac{h}{2}\left.\frac{dx}{dt}\right|_{t+h/2} + \frac{1}{2}\left(\frac{h}{2}\right)^2 \left.\frac{d^2x}{dt^2}\right|_{t+h/2} - ...\right] \\
x(t+h) - x(t) &= h\left.\frac{dx}{dt}\right|_{t+h/2} + \mathcal{O}(h^3) \\
x(t+h) - x(t) &= hf(x(t+h/2), t+h/2) + \mathcal{O}(h^3) \\
x(t+h) &= x(t) + hf(x(t+h/2), t+h/2) + \mathcal{O}(h^3) \\
x(t+h) &\approx x(t) + hf(x(t+h/2), t+h/2) \qquad (10)
\end{aligned}
$$

This looks better than Euler's method, since the leader-order error in Euler's method was of order h^2, and here the leading-order error is of order h^3. But we have a problem - we don't know the value $x(t + h/2)$. (Remember, we start out knowing f and the value of x at one value of t. The formula above requires us to know x at two values, t and $t + h/2$.)

The solution is to approximate the value $x(t+h/2)$ using Euler's method, with $h \to h/2$ in Equation 4.

$$x(t+h/2) \approx x(t) + \frac{h}{2} f(x,t) \tag{11}$$

So we have

$$\begin{aligned} x(t+h) &\approx x(t) + hf(x(t+h/2), t+h/2) \\ x(t+h) &\approx x(t) + hf\left(\left[x + \frac{h}{2} f(x,t)\right], t+h/2\right) \end{aligned} \tag{12}$$

which is easier to write in multiple steps:

$$k_1 = hf(x,t) \tag{13}$$

$$k_2 = hf(x + \frac{1}{2}k_1, t+h/2) \tag{14}$$

$$x(t+h) \approx x(t) + k_2 \tag{15}$$

Now since we used Euler's method to approximate $x(t+h/2)$ instead of using the true value, we have introduced additional error into the calculation. Let's expand the function $f(x+k_1/2, t+h/2)$ using Equation 2 with $z = x(t) + k_1/2$ and $a = x(t+h/2)$ (an expansion in x, ignore t-dependence of f):

$$\begin{aligned} f(x+k_1/2) &= \sum_{i=0}^{\infty} \frac{f^{(i)}(x(t+h/2))}{i!} (x(t) + k_1/2 - x(t+h/2))^i \\ f(x+k_1/2) &= f(x(t+h/2)) + [x(t) + k_1/2 - x(t+h/2)] \left.\frac{\partial f}{\partial x}\right|_{x(t+h/2)} \\ &\quad + \mathcal{O}([x(t) + k_1/2 - x(t+h/2)]^2) \end{aligned} \tag{16}$$

Recall our definition of Euler's rule:

$$x(t+h) = x(t) + hf(x,t) + \mathcal{O}(h^2) \tag{17}$$

If we take $h \to h/2$, substitute with k_1 where appropriate, and rearrange, we have

$$\begin{aligned} x(t+h/2) &= x(t) + \frac{h}{2} f(x,t) + \mathcal{O}(h^2) \\ x(t+h/2) &= x(t) + \frac{k_1}{2} + \mathcal{O}(h^2) \\ -x(t) - \frac{k_1}{2} + x(t+h/2) &= \mathcal{O}(h^2) \\ x(t) + \frac{k_1}{2} - x(t+h/2) &= \mathcal{O}(h^2) \end{aligned} \tag{18}$$

Plugging this into our expansion for f above:

$$\begin{aligned} f(x+k_1/2) &= f(x(t+h/2)) + \mathcal{O}(h^2) \left.\frac{\partial f}{\partial x}\right|_{x(t+h/2)} + \mathcal{O}((h^2)^2) \\ f(x+k_1/2) &= f(x(t+h/2)) + \mathcal{O}(h^2) \end{aligned} \tag{19}$$

Let's put the t-dependence back in now:

$$f(x + k_1/2, t + h/2) = f(x(t + h/2), t + h/2) + \mathcal{O}(h^2) \tag{20}$$

Let's look at the expression for k_2:

$$\begin{aligned}
k_2 &= hf(x + \frac{1}{2}k_1, t + h/2) \\
k_2 &= h\left(f(x(t + h/2), t + h/2) + \mathcal{O}(h^2)\right) \\
k_2 &= hf(x(t + h/2), t + h/2) + \mathcal{O}(h^3)
\end{aligned} \tag{21}$$

And finally look at our expression for $x(t + h)$ again:

$$\begin{aligned}
x(t + h) &= x(t) + hf(x(t + h/2), t + h/2) + \mathcal{O}(h^3) \\
x(t + h) &= x(t) + \left(k_2 + \mathcal{O}(h^3)\right) + \mathcal{O}(h^3) \\
x(t + h) &= x(t) + k_2 + \mathcal{O}(h^3)
\end{aligned} \tag{22}$$

Bottom line: Yes, using Euler's method to do an approximation within our second-order Runge-Kutta (RK2) method does introduce additional error, but the error introduced is also of order h^3, so the overall leading order error is still of order h^3. (If using Euler's method had introduced an error of order h or h^2, then the leading-order error on the RK2 method would become h or h^2 instead of h^3, making RK2 not any better than the simpler Euler method. But that didn't happen, so RK2 has a smaller leading-order approximation error than Euler.)

So why is RK2 better than Euler? See Figure 1. When you use Euler's method, you use the slope of the function at $t = t_0$ to extrapole a line to $t_0 + h$; the value of the linear function at that point is your approximation for $x(t_0 + h)$. With RK2, you use the slope of the function at $t = t_0 + h/2$ to extrapolate a line to $t_0 + h$; the value of that linear function is your approximation for $x(t_0 + h)$.

Example: Second-order RK

3 The Fourth-Order Runge-Kutta Method

As mentioned above, the Runge-Kutta method is actually a set of methods. We've seen the first-order Runge-Kutta (Euler's method) and the second-order Runge-Kutta (RK2). In general, RK approximations estimate the slope by a weighted average of serveral terms of the form $f(x_i, t_i)$, where the t_i are values between t and $t + h$. The x_i are determined by using the Euler method (or some similar method). The most commonly used approximation

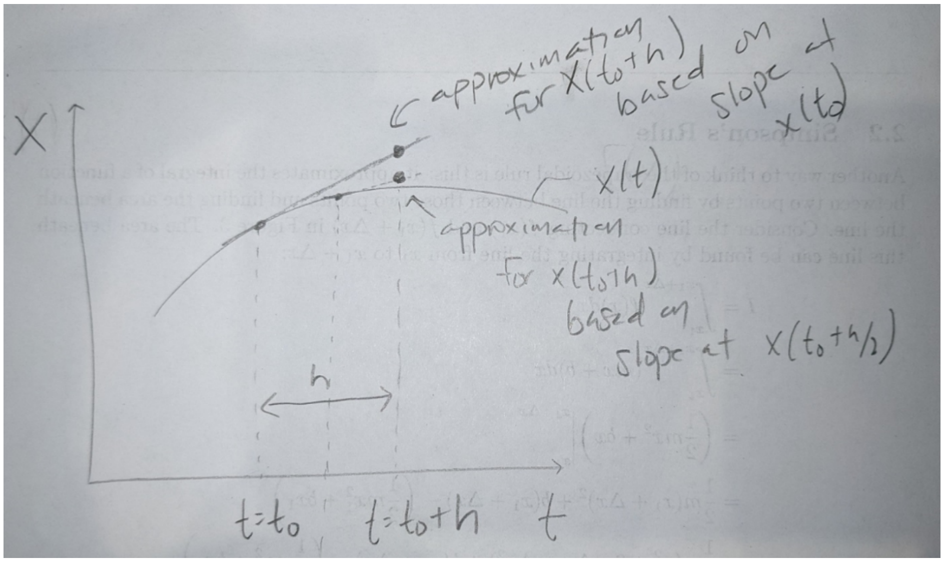

Figure 1:

is the fourth-order RK (RK4) defined like this:

$$k_1 = hf(x,t) \tag{23}$$
$$k_2 = hf(x + k_1/2, t + h/2) \tag{24}$$
$$k_3 = hf(x + k_2/2, t + h/2) \tag{25}$$
$$k_4 = hf(x + k_3, t + h) \tag{26}$$
$$x(t+h) = x(t) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \tag{27}$$

We won't go through the detailed derivation, but it proceeds roughly the same as the derivation for the RK2, just with more algebra. RK4 is accurate to order h^5.

Example: Fourth-order RK

4 Infinite ranges

Suppose you are solving a time-dependent differential equation where $t \to \infty$. We can't use the methods above directly, since it would require an infinite number of steps. However, we can use the methods above if we first apply a change of variable. Note that this also works for numerical integration over infinite ranges. For a range of t from 0 to ∞, use the change of variable:

$$u = \frac{t}{1+t} \tag{28}$$

When $t = 0$, $u = 0$, but when $t \to \infty$, $u \to 1$. Solving for t, we have

$$\begin{aligned}
t &= \frac{u}{1-u} \qquad (29)\\
\frac{dt}{du} &= \frac{u}{(1-u)^2} + \frac{1}{1-u}\\
&= \frac{u}{(1-u)^2} + \frac{1-u}{(1-u)^2}\\
&= \frac{1}{(1-u)^2} \qquad (30)
\end{aligned}$$

If we have a differential equation $\frac{dx}{dt} = f(x,t)$, we can rewrite it as

$$\begin{aligned}
\frac{dx}{dt} &= f(x,t)\\
\frac{dx}{du}\frac{du}{dt} &= f(x,t)\\
\frac{dx}{du} &= \frac{dt}{du} f(x,t)\\
\frac{dx}{du} &= \frac{1}{(1-u)^2} f\left(x, \frac{u}{1-u}\right) \qquad (31)
\end{aligned}$$

If we let

$$g(x,u) = \frac{1}{(1-u)^2} f\left(x, \frac{u}{1-u}\right) \qquad (32)$$

Then our differential equation becomes

$$\frac{dx}{du} = g(x,u) \qquad (33)$$

where u has finite limits.

Section 3, Exercise 2

5 Extension to other problems

5.1 More than one dependent variable

So far, we have only looked at ordinary differential equations with one dependent variable, x, but some problems will have more than one dependent variable, like x and y. Since we are talking about ordinary differential equations (not partial differential equations), there is still only one independent variable t. For example,

$$\frac{dx}{dt} = xy - x \qquad (34)$$

$$\frac{dy}{dt} = y - xy + \sin^2(\omega t), \qquad (35)$$

where the goal is to solve for $x(t)$ and $y(t)$.

In general, we can represent these problems as

$$\frac{d\vec{r}}{dt} = \vec{f}(\vec{r}, t) \tag{36}$$

where $\vec{r}(t) = (x(t), y(t))$ and $\vec{f} = (f_x(x, y, t), f_y(x, y, t))$.

We can use the methods discussed in previous sections in this case. For example, the Euler method:

$$\vec{r}(t + h) = \vec{r}(t) + h\vec{f}(\vec{r}, t) \tag{37}$$

And the fourth-order Runge-Kutta:

$$\vec{k}_1 = h\vec{f}(\vec{r}, t) \tag{38}$$
$$\vec{k}_2 = h\vec{f}(\vec{r} + \vec{k}_1/2, t + h/2) \tag{39}$$
$$\vec{k}_3 = h\vec{f}(\vec{r} + \vec{k}_2/2, t + h/2) \tag{40}$$
$$\vec{k}_4 = h\vec{f}(\vec{r} + \vec{k}_3, t + h) \tag{41}$$
$$\vec{r}(t + h) = \vec{r}(t) + \frac{1}{6}(\vec{k}_1 + 2\vec{k}_2 + 2\vec{k}_3 + \vec{k}_4) \tag{42}$$

There are more complicated cases, of course. For example, if dx/dt depends on dy/dt, a different method would be required.

5.2 Second-order differential equations

Consider a second-order differential equation given by

$$\frac{d^2x}{dt^2} = f\left(x, \frac{dx}{dt}, t\right) \tag{43}$$

The second derivative of x is given by a function f, which can depend on x, t, and the first derivative of x.

To solve this, define a new dependent variable y, which is given by

$$\frac{dx}{dt} = y \tag{44}$$

Written in terms of y, the second-order differential equation above is given by

$$\frac{dy}{dt} = f(x, y, t) \tag{45}$$

So one second-order differential equation (Equation 43) has been transformed into two simultaneous first-order equations (Equations 44 and 45), which we can solve using the techniques of the previous section. This can be generalized to higher orders (for example, a third-order differential equation can be transformed into three simultaneous first-order equations) and to higher-order equations for more than one dependent variable, i.e.

$$\frac{d^2\vec{r}}{dt^2} = f\left(\vec{r}, \frac{d\vec{r}}{dt}, t\right) \tag{46}$$

becomes

$$\frac{d\vec{r}}{dt} = \vec{s} \tag{47}$$

$$\frac{d\vec{s}}{dt} = f(\vec{r}, \vec{s}, t) \tag{48}$$

In general, a system of n equations of mth order becomes a system of $m \times n$ simultaneous first-order equations.

6 Other Methods

There are of course numerous other methods to solve ordinary differential equations, and we're not going to cover all of them. The Runge-Kutta method is a good, general-use method, but other methods might be more appropriate in certain situations. For example, both the Euler method and Runge-Kutta methods have a feature that can lead to solutions that don't conserve energy. Both methods are "asymmetric" in the sense that if you started at the end point of your calculation and used a time-step of $-h$, you wouldn't recover the starting point, i.e. the predicted value of x at time t_0 would not be x_0. Due to this asymmetry, you can get a solution for a simple harmonic oscillator where the amplitude grows with time, which means energy which grows with time (instead of being constant in time, which is expected with energy conservation). So-called "centered difference methods" are symmetric with $h \to -h$, and can be a better choice for oscillating systems, particularly when you want a solution that covers many periods of the oscillation.

So far we have only considered cases where the time step h is constant. One can get improved results by using adaptive step sizes, taking larger step sizes where the function is varying slowly (flat) and smaller step sizes where the function is varying rapidly (near peaks and valleys for example).