Differential Equations

1. First order differential equations – variables separable

A first order differential equation with variables separable is one of the form:

$$\frac{dy}{dx} = f(x).g(y)$$

i.e.: (1) It only involves **first order** derivatives, i.e. only $\frac{dy}{dx}$, not $\frac{d^2y}{dx^2}$, $\frac{d^3y}{dx^3}$, etc.

(2) The **variables *x* and *y* may be easily separated** to obtain an equation which may be integrated:

$$\frac{1}{g(y)}dy = f(x)dx$$

Q1.1 Find the general solution of the differential equation:

$$\frac{dy}{dx} = xy$$

A1.1 By separating the variables we obtain:

$$\frac{1}{y}dy = xdx$$

which upon integration of both sides we obtain:

$$\int \frac{1}{y}dy = \int xdx$$

$$\ln|y| + c_1 = \frac{x^2}{2} + c_2$$

$$or: \ln|y| = \frac{x^2}{2} + K$$

NOTE: *Since the final solution contains the undermined constant of integration, this solution is referred to as the 'general solution'.*

Q1.2 Given that $y(0)=3$, find the particular solution of the differential equation:

$$\frac{dy}{dx}=\frac{1}{y}\sin(x)$$

A1.2 By separating the variables we obtain:

$$ydy=\sin(x)dx$$

which upon integration of both sides we obtain the general solution:

$$\int ydy=\int\sin(x)dx$$

$$\frac{y^2}{2}=-\cos(x)+K$$

We may now obtain the particular solution by using the fact that $y(0)=3$, i.e. that at x=0, y=3, i.e.:

$$\frac{y^2}{2}=-\cos(x)+K,\quad y(0)=3$$

$$\Rightarrow\ \frac{3^2}{2}=-\cos(0)+K$$

$$\Rightarrow\ \frac{9}{2}=-1+K$$

$$\Rightarrow\ K=1+\frac{9}{2}=\frac{11}{2}$$

i.e. the particular solution is given by:

$$\frac{y^2}{2}=-\cos(x)+\frac{11}{2}\quad or:\quad y^2+2\cos(x)+11=0$$

Q1.3 For a first order chemical reaction, the rate law is given by:

$$\frac{d[\mathrm{A}]}{dt}=-k[\mathrm{A}]$$

Given that at time t=0, the initial concentration of A is given by $[\mathrm{A}]_0$, obtain an expression for, $[\mathrm{A}]_t$, the concentration of A at any time t after the commencement of the reaction.

A1.3 By separating the variables we obtain:

$$\frac{1}{[\mathrm{A}]}d[\mathrm{A}]=-kdt$$

This may be solved in one of two ways (with method B being the recommended method).

Method A: By integration of both sides we obtain the general solution:

$$\int \frac{1}{[\mathrm{A}]} d[\mathrm{A}] = \int -k dt$$

$$\int \frac{1}{[\mathrm{A}]} d[\mathrm{A}] = -k \int dt$$

$$\ln[\mathrm{A}] = -kt + const$$

where $[\mathrm{A}]$ represents the concentration of A at any time *t*. Given that at time *t*=0, the initial concentration of A is given by $[\mathrm{A}]_0$, we may now obtain the particular solution:

$$\ln[\mathrm{A}] = -kt + const, \quad \text{at } t = 0, \ [\mathrm{A}] = [\mathrm{A}]_0$$

$$\Rightarrow \ln[\mathrm{A}]_0 = -k0 + const$$

$$\Rightarrow const = \ln[\mathrm{A}]_0$$

i.e. the particular solution is given by:

$$\ln[\mathrm{A}] = -kt + \ln[\mathrm{A}]_0$$

or: $\ln[\mathrm{A}]_t = -kt + \ln[\mathrm{A}]_0$

i.e.: $\ln[\mathrm{A}] - \ln[\mathrm{A}]_0 = -kt$ or: $\ln\left(\frac{[\mathrm{A}]}{[\mathrm{A}]_0}\right) = -kt$

Method B: By integration of both sides using the appropriate boundary conditions we immediately obtain the general solution:

$$\int_{[\mathrm{A}]_0}^{[\mathrm{A}]_t} \frac{1}{[\mathrm{A}]} d[\mathrm{A}] = \int_0^t -k dt$$

$$\int_{[\mathrm{A}]_0}^{[\mathrm{A}]_0} \frac{1}{[\mathrm{A}]} d[\mathrm{A}] = -k \int_0^t dt$$

$$\Big[\ln[\mathrm{A}]\Big]_{[\mathrm{A}]_0}^{[\mathrm{A}]_t} = -k[t]_0^t$$

$$\ln[\mathrm{A}]_t - \ln[\mathrm{A}]_0 = -k(t-0)$$

i.e.: $\ln[\mathrm{A}]_t - \ln[\mathrm{A}]_0 = -kt$ or: $\ln\left(\frac{[\mathrm{A}]_t}{[\mathrm{A}]_0}\right) = -kt$

2. Second order differential equations, homogeneous with constant coefficients

In general a second order differential equation is of the form:

$$\frac{d^2y}{dx^2} + p(x)\frac{dy}{dx} + q(x)y = r(x)$$

and if $r(x) = 0$, then the solution is said to be **homogeneous**. In this course we shall only deal with homogeneous second order differential equations where $p(x)$ and $q(x)$ are constants, i.e. (in its more general form):

$$a\frac{d^2y}{dx^2} + b\frac{dy}{dx} + cy = 0$$

and it may be shown that such an equation will always have a solution of the from $e^{\lambda x}$ where λ is a suitable constant.

In particular, let $y = e^{\lambda x}$ be a trial solution of the equation:

$$a\frac{d^2y}{dx^2} + b\frac{dy}{dx} + cy = 0$$

From $y = e^{\lambda x}$ we may obtain:

$$\frac{dy}{dx} = \lambda e^{\lambda x} \qquad \text{and} \qquad \frac{d^2y}{dx^2} = \frac{d}{dx^2}\left(\lambda e^{\lambda x}\right) = \lambda^2 e^{\lambda x}$$

By substitution into the differential equation we obtain:

$$\lambda^2 e^{\lambda x} + a\lambda e^{\lambda x} + be^{\lambda x} = 0$$

i.e.:

$$e^{\lambda x}\left(a\lambda^2 + b\lambda + c\right) = 0$$

which since $\forall \lambda x,\ e^{\lambda x} > 0$, we obtain the so called **characteristic equation**:

$$a\lambda^2 + b\lambda + c = 0$$

The characteristic equation is a simple quadratic equation with roots:

$$\lambda = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

or: $$\lambda_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \quad \text{and} \quad \lambda_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a}$$

The nature of these roots depend on the discriminant $b^2 - 4ac$. If *a*, *b* and *c* are real numbers then the three possible types of roots are:

- If $b^2 - 4ac > 0$ (positive), then there are two distinct real roots
- If $b^2 - 4ac = 0$ then there is one double real root
- If $b^2 - 4ac < 0$ (negative), then roots are pair of complex conjugates.

Furthermore,

(1) If $b^2 - 4ac > 0$, i.e. λ_1 and λ_2 are distinct real numbers, then the general solution of the differential equation is $y = Ae^{\lambda_1 x} + Be^{\lambda_2 x}$ where A and B are constants, $\lambda_1 = \dfrac{-b + \sqrt{b^2 - 4ac}}{2a}$ and $\lambda_2 = \dfrac{-b - \sqrt{b^2 - 4ac}}{2a}$;

(2) If $b^2 - 4ac = 0$, i.e. $\lambda_1 = \lambda_2 = -\dfrac{b}{2a}$, then the general solution of the differential equation is $y = (A + B)e^{\lambda x} = (A + Bx)\exp\left(\dfrac{-b}{2a}x\right)$ where A and B are constants.

(3) If $b^2 - 4ac < 0$, then we have:

$$\lambda_1 = \frac{-b}{2a} \pm \frac{\sqrt{b^2 - 4ac}}{2a} = \frac{-b}{2a} \pm \sqrt{\left(\frac{b}{2a}\right)^2 - \left(\frac{b}{a}\right)} = \frac{-b}{2a} \pm i\sqrt{\left|\left(\frac{b}{2a}\right)^2 - \left(\frac{b}{a}\right)\right|} \equiv \alpha \pm i\beta$$

where $\alpha = \dfrac{-b}{2a}$, $\beta = \sqrt{\left|\left(\dfrac{b}{2a}\right)^2 - \left(\dfrac{b}{a}\right)\right|}$. The general solution of the differential equation is hence of the form:

$$\begin{aligned} y &= A\exp\left[(\alpha + i\beta)x\right] + B\exp\left[(\alpha - i\beta)x\right] \\ &= A\exp(\alpha x)\exp(i\omega x) + B\exp(\alpha x)\exp(-i\omega x) \\ &= \exp(\alpha x)\left[Ae^{i\beta x} + Be^{-i\beta x}\right] \end{aligned}$$

or in trigonometric form by recalling that $Re^{i\theta} = R\left[\cos(\theta) + i\sin(\theta)\right]$:

$$\begin{aligned} y &= e^{\alpha x}\left[Ae^{i\beta x} + Be^{-i\beta x}\right] \\ &= e^{\alpha x}\left\{A\left[\cos(\beta x) + i\sin(\beta x)\right] + B\left[\cos(-\beta x) + i\sin(-\beta x)\right]\right\} \\ &= e^{\alpha x}\left\{A\left[\cos(\beta x) + i\sin(\beta x)\right] + B\left[\cos(\beta x) - i\sin(\beta x)\right]\right\} \\ &= e^{\alpha x}\left\{(A + B)\cos(\beta x) + i(A - B)\sin(\beta x)\right\} \\ &\equiv e^{\alpha x}\left\{C\cos(\beta x) + D\sin(\beta x)\right\} \end{aligned}$$

where $\alpha = \dfrac{-b}{2a}$, $\beta = \sqrt{\left|\left(\dfrac{b}{2a}\right)^2 - \left(\dfrac{b}{a}\right)\right|}$ and C and D are constants.

In each case, if initial or boundary conditions are specified, the particular solution is then obtained at the end by determining the values of the constants *A*, *B*, *C* or *D* (as appropriate).

Summary:

Second order differential equations of the form $a\frac{d^2y}{dx^2}+b\frac{dy}{dx}+cy=0$ have a corresponding **characteristic equation** of the form $a\lambda^2+b\lambda+c=0$ which:

1. If the characteristic equation has different real roots λ_1,λ_2 then the general solution is of the form $y=Ae^{\lambda_1 x}+Be^{\lambda_2 x}$
2. If the characteristic equation has equal real roots $\lambda=\lambda_1=\lambda_2$ then the general solution is of the form $y=(A+Bx)e^{\lambda x}$
3. If the characteristic equation has complex conjugate roots $\lambda=\alpha\pm\beta i$, then the general solution is of the form $y=e^{\alpha x}\{C\cos(\beta x)+D\sin(\beta x)\}$

In each case, given the general solution, one may obtain the particular solution (i.e. determine the values of the constants *A*, *B*, *C* or *D* (as appropriate)) provided that initial or boundary conditions are specified.

Q 2.1: Find the particular solution of the following second order differential equation:

$$y''+y'-6y=0$$

given that $y(0)=0,\ y'(0)=5$.

A 2.1: The characteristic equation is $\lambda^2+\lambda-6=0$. This factorises to $(\lambda-2)(\lambda+3)=0$, i.e. the roots of the characteristic equation are $\lambda_1=2,\lambda_2=-3$.

The general solution is hence given by:

$$y=Ae^{2x}+Be^{-3x}$$

The particular solution may be obtained since we know that $y(0)=0,\ y'(0)=5$. Thus since:

$$y'=2Ae^{2x}-3Be^{-3x}$$

i.e. at x = 0:

$$y(0)=0$$

i.e.

$$Ae^0+Be^0=A+B=0 \qquad \text{(eqn. 1)}$$

and:

$$y'(0)=5$$

i.e.

$$2Ae^0-3Be^0=2A-3B=5 \qquad \text{(eqn. 2)}$$

i.e. solving eqn. 1 & 2 simultaneously we have:

$$\left.\begin{array}{l}A+B=0\\2A-3B=5\end{array}\right\}A=1,B=-1$$

i.e. the particular solution is given by:

$$y = e^{2x} - e^{-3x}$$

Note: You may verify that $y = e^{2x} - e^{-3x}$ is indeed the solution for the differential equation through differentiation since:

$$y = e^{2x} - e^{-3x}$$
$$y' = 2e^{2x} + 3e^{-3x}$$
$$y'' = 4e^{2x} - 9e^{-3x}$$

which when substituted into:

$$y'' + y' - 6y = 0$$

we obtain:

$$\begin{aligned} LHS &= \left(4e^{2x} - 9e^{-3x}\right) + \left(2e^{2x} + 3e^{-3x}\right) - 6\left(e^{2x} - e^{-3x}\right) \\ &= 4e^{2x} - 9e^{-3x} + 2e^{2x} + 3e^{-3x} - 6e^{2x} + 6e^{-3x} \\ &= 0 \\ &= RHS \end{aligned}$$

Q 2.2: Find the general solution of the following second order differential equations:

(i) $y'' + 3y' + 2y = 0$

(ii) $2y'' + 8y' + 4y = 0$

(iii) $y'' + 2y' + 1y = 0$

(iv) $y'' + 2y' + 3y = 0$

(v) $y'' + 2y' + 4y = 0$

Q 3.1: *The wave function of a particle in a one-dimensional box:* Solve the Schrödinger equation below to obtain:

(i) acceptable wave function(s), $\psi = \psi(x)$, and

(ii) the corresponding total energy(s), E

for a particle of mass m moving in the x-direction:

$$\hat{H}\psi = E\psi$$

where $\hat{H}$ is the appropriate Hamiltonian that gives the total energy E and is given by:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

and $V(x)$ is the potential energy of the particle which is given by:

$$V(x) = \begin{cases} 0 & 0 < x < l \\ \infty & otherwise \end{cases}$$

given the boundary conditions that:

$$\psi(0) = \psi(l) = 0$$

and that for the wave function to be normalised, the wave function must satisfy the condition:

$$\int_0^l \psi^2(x)\,dx = 1$$

A3.1: The SWE may be written as:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi = E\psi$$

i.e.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

which for the particle inside the box (i.e. $0 < x < l$) we have $V(x) = 0$, i.e.:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

or:

$$\left[\frac{\hbar^2}{2m}\right]\frac{d^2\psi}{dx^2} + [E\ ]\psi = 0$$

This is a homogenous second order differential equation of the form:

$$A\frac{d^2y}{dx^2} + B\frac{dy}{dx} + Cy = 0$$

with a characteristic equation:

$$A\lambda^2 + B\lambda + C = 0$$

i.e. in this case:

$$\left[\frac{\hbar^2}{2m}\right]\lambda^2 + E = 0$$

which re-arranges to:

$$\left[\frac{\hbar^2}{2m}\right]\lambda^2 = -E$$

i.e.:

$$\lambda^2 = -\frac{E}{\left[\frac{\hbar^2}{2m}\right]} = -\frac{2mE}{\hbar^2}$$

i.e.:

$$\lambda = \pm\sqrt{-\frac{2mE}{\hbar^2}} = \pm i\sqrt{\frac{2mE}{\hbar^2}} \equiv \alpha \pm i\beta$$

where: $\alpha = 0, \beta = \sqrt{\frac{2mE}{\hbar^2}}$

Thus the general solution to this equation is given by:

$$y = e^{\alpha x}\left\{C\cos(\beta x) + D\sin(\beta x)\right\}$$

i.e. in this case:

$$\psi(x) = C\cos(\beta x) + D\sin(\beta x)$$

where $\beta = \sqrt{\frac{2mE}{\hbar^2}}$

On application of the boundary condition we obtain that:

$$\psi(0) = 0 \Rightarrow C\cos(0) + D\sin(0) = 0$$

$$C(1) + D(0) = 0$$

i.e. $\quad C = 0$

and:

$$\psi(l) = 0 \Rightarrow D\sin(\beta l) = 0$$

which for $\sin(\beta l) = 0$, we must have:

$$\beta l = n\pi$$

(Recall that $\sin(x) = 0$ for $x = \ldots -3\pi, -2\pi, -\pi, 0, \pi, 2\pi, 3\pi\ldots$.)

i.e.:

$$\beta = \frac{n\pi}{l}$$

i.e.:

$$\psi(x) = D\sin(\beta x) = D\sin\left(\frac{n\pi x}{l}\right)$$

Also, for the for the wave function to be normalised, the wave function must satisfy the condition:

$$\int_0^l \psi^2(x)\,dx = 1$$

i.e.:

$$\int_0^l \left[D^2\sin^2\left(\frac{n\pi x}{l}\right)\right]dx = 1$$

i.e.:

$$D^2 \int_0^l \sin^2\left(\frac{n\pi x}{l}\right) dx = 1$$

where since $\cos 2A = 1 - 2\sin^2 A$ then :

$$\sin^2\left(\frac{n\pi x}{l}\right) = \frac{1}{2}\left[1 - \cos\left(\frac{2n\pi x}{l}\right)\right]$$

i.e. since:

$$\frac{d}{dx}\left(\frac{\sin(Ax)}{A}\right) = \frac{A\cos(Ax)}{A} = \cos(Ax) \Rightarrow \int \cos(Ax)\,dx = \frac{\sin(Ax)}{A} + const$$

then:

$$\int_0^l \sin^2\left(\frac{n\pi x}{l}\right) dx = \frac{1}{2}\int_0^l 1 - \cos\left(\frac{2n\pi x}{l}\right) dx = \frac{1}{2}\left[x - \frac{l}{2n\pi}\sin\left(\frac{2n\pi x}{l}\right)\right]_0^l$$

$$= \frac{1}{2}\left[l - \frac{l}{2n\pi}\sin\left(\frac{2n\pi l}{l}\right)\right] - \left[0 - \frac{l}{2n\pi}\sin(0)\right]$$

$$= \frac{1}{2}[l - 0] - [0 - 0] = \frac{l}{2}$$

which implies that:

$$D^2 \frac{l}{2} = 1$$

i.e.:

$$D^2 = \frac{2}{l}$$

i.e.:

$$D = \sqrt{\frac{2}{l}}$$

Thus the wave-functions are given by:

$$\psi_n(x) = \sqrt{\frac{2}{l}}\sin\left(\frac{n\pi x}{l}\right)$$

Also, the general solution for the SWE suggests that:

$$\beta = \sqrt{\frac{2mE}{\hbar^2}}$$

whilst the boundary conditions require that:

$$\beta = \frac{n\pi}{l}$$

Thus:

$$\beta = \sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{l}$$

i.e.:

$$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{l^2}$$

i.e. the corresponding energies for the wave functions $\psi_n(x)$ are given by:

$$E_n = \frac{n^2\pi^2\hbar^2}{2ml^2} = \frac{n^2h^2}{8ml^2}$$

ASIDE: The Hamiltonian for this system:

The Hamiltonian for this system is given by:

$$\hat{H} = T + V$$

where V and T are the potential and kinetic energy of the particle.

The kinetic energy is given by:

$$T = \frac{1}{2}mv_x^2 = \frac{(mv_x)^2}{2m} = \frac{p_x^2}{2m}$$

and where from Quantum Mechanics:

$$p_x = mv_x = -\frac{ih}{2\pi}\frac{d}{dx}$$

i.e.:

$$T = \frac{1}{2m}\left(-\frac{ih}{2\pi}\frac{d}{dx}\right)^2 = -\frac{h^2}{8\pi^2 m}\frac{d^2}{dx^2} \equiv -\frac{\hbar}{2m}\frac{d^2}{dx^2}$$

where h is Plank's constant and $\hbar = \frac{h}{2\pi}$.

Thus the Hamiltonian is given by:

$$\hat{H} = T + V = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

Also, for a particle in a 1D square well (i.e. for $0 < x < l$), the potential energy is given by:

$$V(x) = \begin{cases} 0 & 0 < x < l \\ \infty & otherwise \end{cases}$$

Thus the Hamiltonian for the particle in the well simplifies to:

$$\hat{H} = T + V = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + 0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

i.e. the SWE is given by:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$