CHEM1034 - Week 22 Lecture – Ordinary Differential Equations, Part III

Sections 12.1-12.5 of Steiner, "The Chemistry Maths Book", 2nd edition.

Definite integrals as functions of the upper limit

If a function $f(t)$ is integrable in some interval $[a,b]$, then it is also integrable in any interval $[a,x]$ where $x \in [a,b]$ and the following function may be defined:

$$\Phi(x) = \int_a^x f(t)\,dt \tag{1}$$

This function is continuous and it is easy to demonstrate that its derivative is equal to $f(x)$:

$$\Phi'(x) = \left[\int_a^x f(t)\,dt\right]' = \left[F(x) - F(a)\right]' = F'(x) = f(x) \tag{2}$$

A number of useful function functions are defined as functions of the upper limit:

$$\begin{gathered} S(x) = \int_0^x \sin(t^2)\,dt, \quad C(x) = \int_0^x \cos(t^2)\,dt \quad \text{- Fresnel functions (optics)} \\ \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\,dt \quad \text{- error function (statistics)} \\ \Gamma(z,a,b) = \int_a^b t^{z-1} e^{-t}\,dt \quad \text{- incomplete gamma function (number theory)} \end{gathered} \tag{3}$$

Because these functions are differentiable with respect to their argument, power series and other approximate expansions may be obtained that allow one to avoid taking a cumbersome integral analytically or numerically. The error function in particular is usually treated as elementary.

Linear second-order ODEs

Consider a differential equation that involves the second, as well as the first, derivative of some function. The general form of an equation that is *linear* with respect to those derivatives is:

$$\frac{d^2y}{dx^2} + p(x)\frac{dy}{dx} + q(x)\,y = r(x) \tag{4}$$

where $p(x)$, $q(x)$ and $r(x)$ are arbitrary functions. In this course we will only consider the case where $p(x)$ and $q(x)$ are constants, and $r(x) = 0$:

$$\frac{d^2y}{dx^2} + a\frac{dy}{dx} + by = 0 \tag{5}$$

It may be demonstrated (the formal proof is outside the scope of this course) that the general solution to this equation has the following form:

$$y(x) = C_1 e^{\lambda_1 x} + C_2 e^{\lambda_2 x} \tag{6}$$

where $\lambda_{1,2}$ depend on a and b, and $C_{1,2}$ are arbitrary constants. For particular solutions, the values of these constants are determined by the boundary conditions. The following procedure is commonly used to solve Equation (5):

1. Use a trial solution of the form $e^{\lambda x}$ to find the values of $\lambda_{1,2}$:

$$\frac{d^2}{dx^2}e^{\lambda x} + a\frac{d}{dx}e^{\lambda x} + be^{\lambda x} = 0 \quad \Rightarrow \quad \lambda^2 e^{\lambda x} + a\lambda e^{\lambda x} + be^{\lambda x} = 0 \quad \Rightarrow \quad \lambda^2 + a\lambda + b = 0 \qquad (7)$$

   The substitution produces a quadratic equation (called *characteristic equation*) and therefore

$$\lambda_{1,2} = \frac{-a \pm \sqrt{a^2 - 4b}}{2} \qquad (8)$$

2. If the two roots are different, then the general solution has the form $y(x) = C_1 e^{\lambda_1 x} + C_2 e^{\lambda_2 x}$. If the two roots are identical, then the general solution has the form $y(x) = C_1 e^{\lambda x} + C_2 x e^{\lambda x}$.

3. To obtain the particular solution, substitute the boundary conditions and solve the resulting system of algebraic equations for the coefficients C_1 and C_2.

4. Check the solution by substituting it back into the differential equation and the initial condition. If both are satisfied, the solution is correct.

5. If the values of $\lambda_{1,2}$ are complex, the solution may optionally be expressed in trigonometric form using Euler's formula:

$$e^{(\alpha + i\beta)x} = e^{\alpha x} e^{i\beta x} = e^{\alpha x}\left[\cos(\beta x) + i\sin(\beta x)\right] \qquad (9)$$

   If the coefficients a and b in the original differential equation are real, this procedure makes complex numbers disappear from the solution.

Example 1: find the general solution of $y'' - 5y' + 6y = 0$ and the particular solution for which $y(0) = 3$ and $y'(0) = 8$.

Solution: using the trial solution $e^{\lambda x}$ produces the following characteristic equation

$$\lambda^2 - 5\lambda + 6 = 0$$

Solving this equation yields $\lambda_1 = 3$ and $\lambda_2 = 3$, meaning that the general solution has the following form:

$$y(x) = C_1 e^{2x} + C_2 e^{3x}$$

The coefficients of the particular solution are obtained from the initial conditions:

$$\begin{cases} C_1 + C_2 = 3 \\ 2C_1 + 3C_2 = 8 \end{cases} \quad \Rightarrow \quad \begin{cases} C_1 = 1 \\ C_2 = 2 \end{cases}$$

And so the particular solution is

$$y(x) = e^{2x} + 2e^{3x}$$

Substitution back into the original equation and initial conditions confirms that this is the correct particular solution.

Example 2: find the general solution of $f''(t) - 4f'(t) + 4f(t) = 0$ and the particular solution for which $f(0) = 1$ and $f'(0) = 5$.

Solution: using the trial solution $e^{\lambda t}$ produces the following characteristic equation

$$\lambda^2 - 4\lambda + 4 = 0$$

Solving this equation yields $\lambda_1 = 2$ and $\lambda_2 = 2$ (two identical roots), meaning that the general solution has the following form:

$$f(t) = C_1 e^{2t} + C_2 t e^{2t}$$

The coefficients of the particular solution are obtained from the initial conditions:

$$\begin{cases} C_1 = 1 \\ 2C_1 + C_2 = 5 \end{cases} \quad \Rightarrow \quad \begin{cases} C_1 = 1 \\ C_2 = 3 \end{cases}$$

And so the particular solution is

$$f(t) = e^{2t} + 3te^{3t}$$

Substitution back into the original equation and initial conditions confirms that this is the correct particular solution.

An example of systems modelling using ODEs

Apart from chemical kinetics, a good example of differential equations playing a role in mathematical modelling is given by equations of population dynamics in biology. Consider a lawn covered with grass, with a population of rabbits and a population of foxes. We shall make the following assumptions:

1. Grass growth rate is constant. Grass death rate has two contributions: one is proportional to the quantity of grass and the other is a second order reaction between rabbits and grass. Therefore

$$\frac{d}{dt}G(t) = k_{\mathrm{gg}} - k_{\mathrm{gd}}G(t) - k_{\mathrm{ge}}R(t)G(t) \tag{10}$$

2. Rabbit population growth rate is proportional to the size of the population and the amount of grass. Rabbit death rate has two contributions: one is proportional to the size of the population and the other is a second-order reaction between rabbits and foxes. Therefore

$$\frac{d}{dt}R(t) = k_{\mathrm{rb}}R(t)G(t) - k_{\mathrm{rd}}G(t) - k_{\mathrm{re}}R(t)F(t) \tag{11}$$

3. Fox population growth rate is proportional to the size of the population and the amount of rabbits. Fox death rate is proportional to the size of the population. Therefore

$$\frac{d}{dt}F(t) = k_{\mathrm{fb}}R(t)F(t) - k_{\mathrm{fd}}F(t) \tag{12}$$

The result is one of the many possible population dynamics models in this system. It is clear that analytical solutions are unlikely to be simple here – too many product terms that are either hard to separate or inseparable. Assuming the following initial conditions and settings:

$$k_{\mathrm{gg}} = 5,\ k_{\mathrm{gd}} = 1,\ k_{\mathrm{ge}} = 1$$

$$k_{\mathrm{rb}} = 1,\ k_{\mathrm{rd}} = 1,\ k_{\mathrm{re}} = 1$$

$$k_{\mathrm{fb}} = 1,\ k_{\mathrm{fd}} = 1$$

$$G(0) = 10,\ R(0) = 1,\ F(0) = 1$$

we can fire up Mathematica and instruct it to solve the system numerically:

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In[23]:= S = NDSolve[{G'[t] == 5 - G[t] - R[t] G[t],
        R'[t] == R[t] G[t] - R[t] - R[t] F[t],
        F'[t] == R[t] F[t] - F[t], G[0] == 10, R[0] == 3,
        F[0] == 3}, {G, R, F}, {t, 0, 6}]
Out[23]=
{{G → InterpolatingFunction[ Domain: {{0., 6.}} Output: scalar ],
  R → InterpolatingFunction[ Domain: {{0., 6.}} Output: scalar ],
  F → InterpolatingFunction[ Domain: {{0., 6.}} Output: scalar ]}}

In[24]:= Plot[{Evaluate[G[t] /. S], Evaluate[R[t] /. S],
       Evaluate[F[t] /. S]}, {t, 0, 6}, PlotRange → All]
Out[24]=
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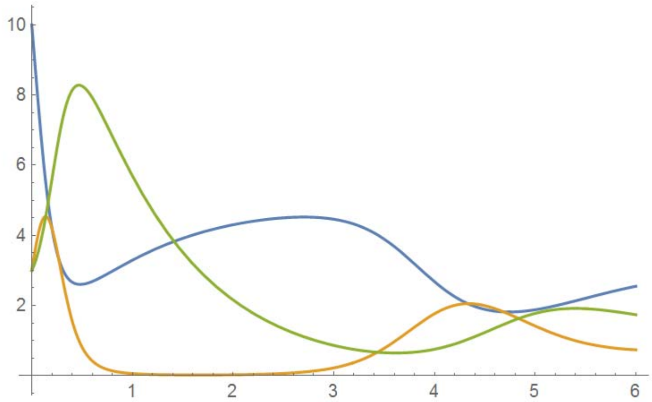

It is clear that the system exhibits some rather complicated behaviour and at some point the poor rabbits very nearly die out. When the equations are solved for an extended period of time, this system settles into the classical oscillating predator-prey dynamics.

Week 23 workshop exercises

Steiner, 2nd edition: section 12.10, problems 1-21.

Extra difficulty exercises for the brave

Steiner, 2nd edition: section 12.10, problems 22, 23.