CHEM2024 – Week 21 Lecture 1 – Ordinary differential equations II

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

1. 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 ODE that is linear with respect to those derivatives is:

$$\frac{d^2y}{dx^2}+p(x)\frac{dy}{dx}+q(x)y=r(x) \tag{1}$$

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 $r(x)=0$:

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

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:

$$y(x)=c_1e^{\lambda_1x}+c_2e^{\lambda_2x} \tag{3}$$

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 initial or the boundary conditions on the function and its first derivative. The following procedure is commonly used to solve Equation (2):

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

   $$\frac{d^2}{dx^2}e^{\lambda x}+a\frac{d}{dx}e^{\lambda x}+be^{\lambda x}=0 \quad\Rightarrow\quad \lambda^2e^{\lambda x}+a\lambda e^{\lambda x}+be^{\lambda x}=0 \quad\Rightarrow\quad \lambda^2+a\lambda+b=0 \tag{4}$$

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

   $$\lambda_{1,2}=\frac{-a\pm\sqrt{a^2-4b}}{2} \tag{5}$$

2. If the two roots are different, then the general solution has the form $y(x)=c_1e^{\lambda_1x}+c_2e^{\lambda_2x}$. If the two roots are identical, then the general solution has the form $y(x)=c_1e^{\lambda_1x}+c_2xe^{\lambda_2x}$.

3. To obtain the particular solution, substitute the initial 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:

   $$e^{(\alpha+i\beta)x}=e^{\alpha x}e^{i\beta x}=e^{\alpha x}\left[\cos(\beta x)+i\sin(\beta x)\right] \tag{6}$$

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

<u>Example 1</u>: 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 $\lambda_1 = 2$ 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:

$$\begin{cases} c_1 + c_2 = 3 \\ 2c_1 + 3c_2 = 8 \end{cases} \Rightarrow \begin{cases} c_1 = 1 \\ c_2 = 2 \end{cases}$$

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:

$$\begin{cases} c_1 = 1 \\ 2c_1 + c_2 = 5 \end{cases} \Rightarrow \begin{cases} c_1 = 1 \\ c_2 = 3 \end{cases}$$

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.

2. Systems of linear first order ODEs

A system of linear first order ODEs has the following general form:

$$\left\{ \frac{df_k(t)}{dt} = a_{k1}(t) f_1(t) + a_{k2}(t) f_2(t) + \ldots \right._k \tag{7}$$

where the k index runs over the equations in the system. In the common case of two equations and constant coefficients:

$$\begin{cases} f_1'(t) = a_{11} f_1(t) + a_{12} f_2(t) \\ f_2'(t) = a_{21} f_1(t) + a_{22} f_2(t) \end{cases} \tag{8}$$

If this system of equations is rewritten in the matrix form:

$$\frac{d}{dt}\begin{pmatrix} f_1(t) \\ f_2(t) \end{pmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{pmatrix} f_1(t) \\ f_2(t) \end{pmatrix} \tag{9}$$

it may be shown (the formal proof is outside the scope of this course) that the general solution is:

$$\begin{pmatrix} f_1(t) \\ f_2(t) \end{pmatrix} = c_1 \vec{v}_1 e^{\lambda_1 t} + c_2 \vec{v}_2 e^{\lambda_2 t} \tag{10}$$

where $\lambda_{1,2}$ are the eigenvalues of the 2×2 matrix, $\vec{v}_{1,2}$ are its eigenvectors, and $c_{1,2}$ are the undetermined coefficients. Note that the eigenvectors do not need to be normalised because the coefficients in front of them are arbitrary anyway.

The plan for solving systems of linear first order ODEs with constant coefficients is therefore as follows:

1. Make the system uniform by any appropriate transformations or substitutions.
2. Rewrite the system in the matrix-vector notation.
3. Obtain the eigenvalues λ_k and eigenvectors $\vec{v}_k$ of the matrix.
4. Write the general solution as $c_1 \vec{v}_1 e^{\lambda_1 t} + c_2 \vec{v}_2 e^{\lambda_2 t} + \ldots$
5. Use the initial conditions to obtain the values of the coefficients and simplify.
6. Check by substituting back into the equations and the initial conditions.

Example 3: find the general solution for the dynamics of a ball of mass m suspended on a spring with stiffness k, for which Newton's equations of motion are:

$$\begin{cases} m\dfrac{d}{dt}v(t) = -k\left[x(t) - x_0\right] \\ \dfrac{d}{dt}x(t) = v(t) \end{cases} \tag{11}$$

and the particular solution for which $x(0) = 0$ and $v(0) = 0$.

Solution: the first equation is non-uniform, but a simple substitution $y(t) = x(t) - x_0$ shifts the reference point and makes it uniform:

$$\begin{cases} \dfrac{d}{dt}v(t) = -\dfrac{k}{m}y(t) \\ \dfrac{d}{dt}y(t) = v(t) \end{cases} \tag{12}$$

The matrix form of this differential equation is:

$$\frac{d}{dt}\begin{bmatrix} v(t) \\ y(t) \end{bmatrix} = \begin{bmatrix} 0 & -k/m \\ 1 & 0 \end{bmatrix} \begin{bmatrix} v(t) \\ y(t) \end{bmatrix} \tag{13}$$

The eigenvalues and eigenvectors of the matrix may be computed in the standard way:

$$\lambda_{1,2} = \pm i\sqrt{\frac{k}{m}}, \qquad \vec{v}_{1,2} = \begin{bmatrix} \pm i\sqrt{k/m} \\ 1 \end{bmatrix} \tag{14}$$

It is useful to denote $\omega = \sqrt{k/m}$. The general solution therefore has the form:

$$\begin{bmatrix} v(t) \\ y(t) \end{bmatrix} = c_1 \begin{bmatrix} +i\omega \\ 1 \end{bmatrix} \exp(+i\omega t) + c_2 \begin{bmatrix} -i\omega \\ 1 \end{bmatrix} \exp(-i\omega t) \tag{15}$$

We can now impose the initial conditions. From the fact that $y(0) = -x_0$ we can conclude that $c_1 + c_2 = -x_0$. From the fact that the initial velocity is zero, we conclude that $c_1 = c_2$. This fixes the values of the two constants and simplifies the solution in Equation (15):

$$\begin{bmatrix} v(t) \\ y(t) \end{bmatrix} = -\frac{x_0}{2} \begin{bmatrix} +i\omega \\ 1 \end{bmatrix} \exp(+i\omega t) - \frac{x_0}{2} \begin{bmatrix} -i\omega \\ 1 \end{bmatrix} \exp(-i\omega t) \tag{16}$$

We can use the standard relations from the complex numbers lecture

$$\begin{aligned} \exp(-i\omega t) + \exp(+i\omega t) &= 2\cos(\omega t) \\ \exp(-i\omega t) - \exp(+i\omega t) &= 2i\sin(\omega t) \end{aligned} \tag{17}$$

to simplify the solution further:

$$\begin{bmatrix} v(t) \\ y(t) \end{bmatrix} = x_0 \begin{bmatrix} \omega\sin(\omega t) \\ -\cos(\omega t) \end{bmatrix} \tag{18}$$

Rewriting this expression in the component notation and reversing the substitution produces the final answer:

$$\begin{cases} x(t) = x_0 - x_0\cos(\omega t) \\ v(t) = x_0\omega\sin(\omega t) \end{cases} \tag{19}$$

<u>Example 4</u>: the system of kinetic equations we have obtained for THC and its metabolites in one pf the previous lectures was

$$\frac{d}{dt}\begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} -k_1 & 0 & 0 \\ +k_1 & -k_2 & 0 \\ 0 & +k_2 & -k_3 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} \tag{20}$$

<u>Solution</u>: to solve this equation, we must calculate the eigenvalues of the matrix:

$$\det\begin{bmatrix} -k_1-\lambda & 0 & 0 \\ +k_1 & -k_2-\lambda & 0 \\ 0 & +k_2 & -k_3-\lambda \end{bmatrix} = 0 \quad \Rightarrow \quad \begin{cases} \lambda_1 = -k_1 \\ \lambda_2 = -k_2 \\ \lambda_3 = -k_3 \end{cases}$$

and the corresponding eigenvectors (not normalised):

$$\vec{v}_1 = \begin{bmatrix} (k_1-k_2)(k_1-k_3)/k_1k_2 \\ (k_3-k_1)/k_2 \\ 1 \end{bmatrix}, \qquad \vec{v}_2 = \begin{bmatrix} 0 \\ (k_3-k_2)/k_2 \\ 1 \end{bmatrix}, \qquad \vec{v}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

Calculating these vectors is a long story, and the normalisation is unnecessary because the coefficients in front of these vectors are variable anyway. After assembling the general solution, we get:

$$\begin{bmatrix} A(t) \\ B(t) \\ C(t) \end{bmatrix} = c_1 \vec{v}_1 e^{-k_1 t} + c_2 \vec{v}_2 e^{-k_2 t} + c_3 \vec{v}_3 e^{-k_3 t} \tag{21}$$

The final answers are:

$$\begin{aligned} A(t) &= A_0 e^{-k_1 t} \\ B(t) &= \frac{A_0 k_1}{k_1 - k_2}\left(e^{-k_2 t} - e^{-k_1 t}\right) \\ C(t) &= \frac{A_0 k_1^2 k_2}{(k_1 - k_2)(k_1 - k_3)(k_2 - k_3)}\left(e^{-k_3 t} - e^{-k_2 t}\right) + \\ &\quad + \frac{A_0 k_1 k_2^2}{(k_1 - k_2)(k_1 - k_3)(k_2 - k_3)}\left(e^{-k_3 t} - e^{-k_1 t}\right) + \\ &\quad + \frac{A_0 k_1 k_2 k_3}{(k_1 - k_2)(k_1 - k_3)(k_2 - k_3)}\left(e^{-k_2 t} - e^{-k_1 t}\right) \end{aligned} \tag{22}$$