Chem237: Lecture 17

Alan Robledo

5/15/18

Solving Linear ODEs using Matrix Methods

We've already discussed solving ODEs (Ordinary Differential Equations) in previous lectures as well as performing an eigenvalue decomposition. Therefore, it makes sense to discuss how we can combine the two topics. We will start with a quick example of a first-order ODE,

$$\dot{y} = ay \quad ; \quad y = y(t) \tag{1}$$

where we are adopting the dot notation from physics where a dot represents a derivative taken with respect to time, e.g. $\dot{y} = \frac{dy}{dt}$, for simplicity.

By inspection, the solution space is one dimension and has the form

$$y = y_o e^{at} \tag{2}$$

where a is a scalar and y_o would be determined from intitial conditions.

We can consider generalizing this by considering an array of functions

$$\vec{Y}(t) = \begin{bmatrix} y_1(t) \\ \vdots \\ y_n(t) \end{bmatrix} \tag{3}$$

and a matrix of coefficients $\mathbf{A}$

$$\begin{bmatrix} A_{11} & \cdots & A_{n1} \\ \vdots & & \vdots \\ A_{1n} & \cdots & A_{nn} \end{bmatrix} \tag{4}$$

such that the following equation is satisfied

$$\dot{Y}(t) = \mathbf{A}Y(t). \tag{5}$$

It is implied that $Y = \vec{Y}$. Equation 5 looks very similar to the Time-Dependent Schrödinger Equation (TDSE),

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi \tag{6}$$

and, without using any quantum mechanics jargon, we can compare this to equation 1 and say that the solution to the TDSE is,

$$\Psi = \psi_o e^{-\frac{it}{\hbar}\hat{H}} \tag{7}$$

If this does bother you then we'll just assume that ψ_o is a stationary state. Going back to equation 5, we can automatically see that the solution looks like,

$$Y(t) = e^{\mathbf{A}t}Y_o \tag{8}$$

where $Y_o = \begin{bmatrix} y_1(0) \\ \vdots \\ y_n(0) \end{bmatrix}$. If we perform an eigenvalue decomposition on $\mathbf{A}$, then we get,

$$\mathbf{A} = \mathbf{X}\Lambda\mathbf{X}^{-1} \tag{9}$$

And using this with equation 8 gives

$$Y(t) = \mathbf{X}e^{\Lambda t}\mathbf{X}^{-1}Y_o \tag{10}$$

1

where we recall that $\mathbf{X}$ is a matrix of eigenvectors and Λ is a diagonal matrix of the eigenvalues. Remember that Y_o is a vector and not a scalar, so it is important to keep it on the right hand side of the equation so that the dimensions are aligned properly.

If you think that there was a big jump between equation 9 and equation 10, we are simply taking the idea from lecture 14 that $\mathbf{A}$ and $e^{\mathbf{A}}$ share the same eigenvectors while the eigenvalues of $\mathbf{a}$ and $e^{\mathbf{A}}$ are λ_n and e^{λ_n} respectively (see lecture 14 for the proof). Likewise, if we mutliply $\mathbf{A}$ by a scalar, t, then $\mathbf{A}t$ and $e^{\mathbf{A}t}$ will share the same eigenvectors while the eigenvalues of $\mathbf{A}t$ and $e^{\mathbf{A}t}$ are $\lambda_n t$ and $e^{\lambda_n t}$ respectively, since scalar multiplication does not change the eigenvectors only the eigenvalues. Therefore, using right multiplication,

$$e^{\mathbf{A}t}\mathbf{X} = \mathbf{X}e^{\Lambda t} \quad \Rightarrow \quad e^{\mathbf{A}t} = \mathbf{X}e^{\Lambda t}\mathbf{X}^{-1} \tag{11}$$