Biophysics and Physiological Modeling

Extract from

Chapter 3: Finite difference method and O_2

Q.3.16 Using the equation you just derived and definition of u (3.10) *show that*

$$\delta u = -2ku\delta t \tag{3.14}$$

…which is the finite difference equation for u that we were looking for.

If we make δt **infinitesimally small** (i.e. extremely small), the solution to equation (3.14) can be found using **calculus** to give the following formula for u as a function of time.

$$u = u_0 e^{-2kt} \tag{3.15}$$

where u_0 is the value of u at time $t = 0$. We can use this equation to calculate u … using a calculator at any time we like… no need to write a spreadsheet. Obviously, if we can find an **analytical solution** like equation (3.15) then it is *definitely* preferable to a FD solution. However, analytical solutions are only available for very simple problems. As we'll see later, more complex problems (like diffusion) can be solved in Excel using FD methods even though no *simple* analytical solution *has ever been found*!

About what you discovered: calculus solution for $u(t)$

This section is included for students who have taken a year of calculus at the university level. If you haven't taken calculus you can skip this derivation… its main purpose is to show how the analytical solution (3.15) can be derived from the FD equation (3.14) using basic calculus. This is actually a very cool and useful mathematical trick that shows why calculus is definitely worth taking if you have the time and the inclination.

If you have taken calculus, the following section shows one of the few problems in biophysics and physiology that can be solved exactly using calculus. Luckily it's one that is both important and ubiquitous (common) – first-order kinetics – as seen in drug elimination, radioactive decay, etc…

In the traditional chemistry approach, calculus is used to model chemical kinetics. We can get to the calculus formulation of our two-box simulation by starting with the finite difference equation we derived above

$$\delta u = -2ku\delta t \tag{3.14}$$

Dividing both sides of equation (3.14) by δt gives

$$\frac{\delta u}{\delta t} = -2ku \tag{3.16}$$

Taking the limit $\delta t \to 0$ results in the **derivative** of u with respect to time t

$$\lim_{\delta t\to 0}\frac{\delta u}{\delta t} = \frac{\mathrm{d}u}{\mathrm{d}t} \tag{3.17}$$

Substituting this limit into equation (3.16) produces the **differential equation**,

$$\frac{\mathrm{d}u}{\mathrm{d}t} = -2ku \tag{3.18}$$

Multiplying both sides by $\mathrm{d}t$ and dividing by u gives

$$\frac{\mathrm{d}u}{u} = -2k\mathrm{d}t \tag{3.19}$$

Integrating from $t = 0$ (and $u = u_0$) to up to time t

$$\int_{u_0}^{u}\frac{\mathrm{d}u'}{u'} = \int_0^t -2k\mathrm{d}t' \tag{3.20}$$

where u' and t' are dummy variable versions of u and t. Evaluating the integrals gives

$$[\ln u']_{u_0}^{u} = [-2kt']_0^t \tag{3.21}$$

Substituting in the limits,

$$\ln u - \ln u_0 = -2kt - (-2k\cdot 0) \tag{3.22}$$

and the dummy variables disappear. Using the property of logs that $\ln u - \ln u_0 = \ln\frac{u}{u_0}$, we get

$$\ln\frac{u}{u_0} = -\,2kt \tag{3.23}$$

Taking e^x of both sides gives

$$\frac{u}{u_0} = e^{-2kt} \tag{3.24}$$

Rearranging gives

$$u = u_0 e^{-2kt} \tag{3.15}$$

which is the equation we were trying to derive… and we're done! Phew… that took a while, but we successfully derived an **analytical solution** (an algebraic equation) for the ensemble average value of u as a function of time for the two-box system. This analytical solution is a **predetermined function** of time. ❑

About what you discovered: connection with Calculus I

Equation (3.17) is exactly the same as the derivative you learned about in Calculus I. However, students sometimes have trouble seeing that because the notation in their calculus textbook is different. In calculus textbooks the **derivative** of a function $f(x)$ is often written as

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \tag{3.25}$$

This equation really doesn't look much like equation (3.17), so let's go over how they match up.

h is a small step in x, so we would change $h \longmapsto \delta x$

$$f'(x) = \lim_{\delta x \to 0} \frac{f(x+\delta x) - f(x)}{\delta x} \tag{3.26}$$

Changing to Leibniz notation: $f'(x) \longmapsto \frac{\mathrm{d}y}{\mathrm{d}x}$; $f(x) \longmapsto y(x)$; and $f(x+\delta x) \longmapsto y(x+\delta x)$

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \lim_{\delta x \to 0} \frac{y(x+\delta x) - y(x)}{\delta x} \tag{3.27}$$

Finally, $y(x+\delta x) - y(x)$ is a small change in y corresponding to a small change in x. Hence, $y(x+\delta x) - y(x) = \delta y$, and equation (3.25) becomes

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \lim_{\delta x \to 0} \frac{\delta y}{\delta x} \tag{3.28}$$

which is exactly the same form as equation (3.17). As you know from Calculus I, the derivative $\frac{\mathrm{d}y}{\mathrm{d}x}$ is the slope of a graph of y versus x. As we'll see below, if we make δt small enough in our FD method we'll approach the calculus answer as $\delta t \to 0$. Hence, the FD method should give the same answer as the analytical solution (3.15) that we derived using the derivative in equation (3.17).

Note: We are using δy for a change in y that *must be small* and we're reserving Δy for a big change or difference. However, you should note that most math and physics textbooks use uppercase Δx and Δy in equations (3.26), (3.27) and (3.28) because they do not make that distinction. ❑

About what you discovered: three "d"s

We now have three "d"s for a change or difference in y (or x or t etc.). Δy is a change or difference in y that does not need to be small, e.g. the difference in height between sea level and the top of Mt. Everest. δy is a change or difference in y that must be small, e.g. the height increase for your first step up the mountain (think a small piece of Δy). $\mathrm{d}y$ is the infinitesimal piece of y that we get if we take the limit $\delta y \to 0$. It is useful to think of each of them as a step in y. Δy is a big step, δy is a small step, and $\mathrm{d}y$ is an infinitesimal increment. ❑

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