Solutions - Partial Differential Equation Models for Biological Processes

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These are partial solutions to exercises posed in the chapter *Partial Differential Equation Models for Biological Processes*. If you find any typos, please email sdolson@wpi.edu.

Solutions to Exercises

1. (a) (1) $\partial f/\partial x = -3y+2x$, $\partial f/\partial y = 2y-3x$.
   (2) $\nabla f = [-3y+2x,\ 2y-3x]$.
   (3) $\Delta f = 4$.
   (b) (1) $\partial f/\partial x = 1/y$, $\partial f/\partial y = -x/y^2$.
   (2) $\nabla f = \left[1/y,\ -x/y^2\right]$.
   (3) $\Delta f = 2x/y^3$.
   (c) (1) $\partial f/\partial x = \cos x \sin y \sin z$, $\partial f/\partial y = \sin x \cos y \sin z$, $\partial f/\partial z = \sin x \sin y \cos z$.
   (2) $\nabla f = [\cos x \sin y \sin z,\ \sin x \cos y \sin z,\ \sin x \sin y \cos z]$.
   (3) $\Delta f = -3 \sin x \sin y \sin z$.
   (d) (1) $\partial f/\partial x = yz$, $\partial f/\partial y = xz$, $\partial f/\partial z = xy$.
   (2) $\nabla f = [yz,\ xz,\ xy]$.
   (3) $\Delta f = 0$.
2. (a) Assume that Ω is an arbitrary domain that the fluid occupies. The mass entering though the surface of this domain $\partial\Omega$ is $J(\mathbf{x},t) = -\rho\mathbf{u}\cdot\hat{\mathbf{n}}$, where $\hat{\mathbf{n}}$ is the unit out normal to the boundary $\partial\Omega$. According to the conservation law of mass,
   $$\frac{d}{dt}\iiint_\Omega \rho d\mathbf{x} = \oiint_{\partial\Omega} -\rho\mathbf{u}\cdot\mathbf{n}dS.$$
   Applying the divergence theorem to the right hand side, we obtain
   $$\iiint_\Omega \frac{\partial\rho}{\partial t}d\mathbf{x} = \iiint_\Omega -\nabla\cdot(\rho\mathbf{u})d\mathbf{x}.$$
   Since Ω is arbitrary, the integral equation above is the same as
   $$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0.$$
   (b) Rewriting $Vol(V_t)$ as an integral and taking $f=1$ in the Reynold transport theorem, we get
   $$\frac{dVol(V_t)}{dt} = \frac{d}{dt}\int_{V_t} dV = \int_{V_t} \nabla\cdot\mathbf{u}dV. \tag{1}$$

Assuming that $\nabla \cdot \mathbf{u}$ is a constant,

$$\frac{dVol(V_t)}{dt} = \int_{V_t} \nabla \cdot \mathbf{u} dV = (\nabla \cdot \mathbf{u}) \int_{V_t} dV = (\nabla \cdot \mathbf{u})\, Vol(V_t). \tag{2}$$

(c) Since the fluid is incompressible, $\nabla \cdot \mathbf{u} = 0$. Combining with the result of part (b), we reach that $\frac{dVol(V_t)}{dt} = 0$, which implies that the volume remains the same in time.

(d) Consider an arbitrary fluid parcel V_t, the rate of change of the mass in this parcel is zero since there is no source or sink, i.e.

$$\frac{d}{dt} \int_{V_t} \rho dV = 0. \tag{3}$$

Replacing f by the density ρ in the Reynold transport theorem, we obtain

$$\frac{d}{dt} \int_{V_t} \rho dV = \int_{V_t} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u})\, dV. \tag{4}$$

Combining the above two identities,

$$\int_{V_t} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u})\, dV = 0. \tag{5}$$

Since V_t is an arbitrary domain, we have

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0. \tag{6}$$

3a. $p(x_i, t_j + \triangle t) = p(x_i, t_j) + \mathcal{P}_R p(x_i - \triangle x, t_j) - \mathcal{P}_L p(x_i, t_j) - \mathcal{P}_R p(x_i, t_j) + \mathcal{P}_L p(x_i + \triangle x, t_j)$

b. $p(x + \triangle x, t) = p(x,t) + p_x \triangle x + 0.5 p_{xx} \triangle x^2 + \cdots,$
rewriting: $p(x_i, t_j + \triangle t) - p(x_i, t_j) = \frac{\triangle x^2}{2} p_{xx}$.

c. When dividing both sides by $\triangle t \to 0$, $p_t = \mathcal{D} p_{xx}$ where $\mathcal{D} = 2 \triangle x^2 / \triangle t$. This corresponds to a Brownian particle moving with constant diffusion and zero drift. Note that if we had assumed $\mathcal{P}_R \neq \mathcal{P}_L$, we would obtain the advection-diffusion equation. For a detailed derivation of the diffusion equation see [1] and see [2] for more information regarding the derivation of the Fokker-Plank equation, which is similar to the diffusion equation, with the addition of an advective term due to random forces.

4. The term on the left is the rate of change of the population density with respect to time. The first term on the right hand side is the diffusive flux of the population; the population will tend to move from regions of higher concentration to regions of lower concentration with diffusive parameter $\mathcal{D}$. This could correspond to organisms spreading out in order to have space or to have access to resources such as food. The second term on the right hand side is a reaction term (local sink or source) corresponding to logistic growth. The parameter K is the carrying capacity, the population density that the organism can survive at with enough resources. If the population density at a given location is greater than the carrying capacity, the term will act as a local sink, causing the population to decrease which could be due to lack of food at this high population density.

5a. Setting $\partial c/\partial t = 0$ and evaluating the divergence of the gradient gives

$$0 = \mathcal{D}\frac{\partial^2 c}{\partial x^2}, \qquad 0 \le x \le L, \tag{7}$$

with Dirichlet boundary conditions $c(0) = c_i$ and $c(L) = c_e$. Integrating (7) two times with respect to x gives $c(x) = k_1 x + k_2$ and invoking the boundary conditions, we arrive at the solution:

$$c(x) = \frac{c_e - c_i}{L}x + c_i.$$

This gives the concentration profile through the pore at steady state.

b. The flux is $J = -\mathcal{D}c_x = -\mathcal{D}(c_e - c_i)/L$, proportional to the concentration difference. We can think of the constant $\mathcal{D}/L$ as the pore permeability for the given chemical.

6. The Fluxes:

$$\mathbf{J} = \mathbf{J}_{\mathcal{D}} + \mathbf{J}_{\mathcal{E}} = -\mathcal{D}\nabla c - \xi c \nabla \psi = 0$$

In 1-d with constant electric potential: $0 = \mathcal{D}\frac{dc}{dx} - \xi c \frac{d\psi}{dx} = 0$
Rewriting assuming $c(x) \neq 0$ and then integrating:

$$\mathcal{D}\int_0^L \frac{1}{c}\frac{dc}{dx}dx + \xi \int_0^L \frac{d\psi}{dx}dx = 0$$

Let $x = 0$ correspond to the inner cell membrane (bordering the intracellular concentration c_i) and let $x = L$ correspond to the exterior boundary of the cell membrane (bordering the extracellular concentration c_e). Then:

$$\ln(c_e) - \ln(c_i) = \frac{zF}{RT}(\psi_e - \psi_i) = \frac{zF}{RT}V$$

where V is the potential difference across the membrane. Thus, $V = \dfrac{RT}{zF}\ln\left(\dfrac{c_e}{c_i}\right)$, which is known as the Goldman-Hodgkin-Katz voltage equation.

7. (a) From the assumption that $c(\mathbf{x}, t)$ is a radially symmetric function with respect to ρ, i.e. $\partial c/\partial \theta = 0$ and $\partial c/\partial \phi = 0$. By the chain rule,

$$\frac{\partial c}{\partial x} = \frac{\partial c}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial c}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial c}{\partial \phi}\frac{\partial \phi}{\partial x} = \frac{\partial c}{\partial \rho}\frac{\partial \rho}{\partial x} = \frac{\partial c}{\partial \rho}\frac{x}{\rho} \tag{8}$$

where $\rho = \sqrt{x^2 + y^2 + z^2}$. Similarly, we can find that

$$\frac{\partial c}{\partial y} = \frac{\partial c}{\partial \rho}\frac{y}{\rho} \quad \text{and} \quad \frac{\partial c}{\partial z} = \frac{\partial c}{\partial \rho}\frac{z}{\rho}. \tag{9}$$

Differentiate $\partial c/\partial x$, $\partial c/\partial y$ and $\partial c/\partial z$ again with respect to x, y and z respectively,

$$\begin{aligned}\frac{\partial^2 c}{\partial x^2} &= \frac{\partial^2 c}{\partial \rho^2}\left(\frac{x}{\rho}\right)^2 + \frac{\partial c}{\partial \rho}\frac{1}{\rho} - \frac{\partial c}{\partial \rho}\frac{x^2}{\rho^3}\\ \frac{\partial^2 c}{\partial y^2} &= \frac{\partial^2 c}{\partial \rho^2}\left(\frac{y}{\rho}\right)^2 + \frac{\partial c}{\partial \rho}\frac{1}{\rho} - \frac{\partial c}{\partial \rho}\frac{y^2}{\rho^3}\\ \frac{\partial^2 c}{\partial z^2} &= \frac{\partial^2 c}{\partial \rho^2}\left(\frac{z}{\rho}\right)^2 + \frac{\partial c}{\partial \rho}\frac{1}{\rho} - \frac{\partial c}{\partial \rho}\frac{z^2}{\rho^3}\end{aligned} \tag{10}$$

Therefore,

$$\begin{aligned}0 = \Delta c &= \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\\ &= \frac{\partial^2 c}{\partial \rho^2}\left(\frac{x}{\rho}\right)^2 + \frac{\partial^2 c}{\partial \rho^2}\left(\frac{y}{\rho}\right)^2 + \frac{\partial^2 c}{\partial \rho^2}\left(\frac{z}{\rho}\right)^2 + \frac{\partial c}{\partial \rho}\frac{3}{\rho} - \left(\frac{\partial c}{\partial \rho}\frac{x^2}{\rho^3} + \frac{\partial c}{\partial \rho}\frac{y^2}{\rho^3} + \frac{\partial c}{\partial \rho}\frac{z^2}{\rho^3}\right)\\ &= \frac{\partial^2 c}{\partial \rho^2} + \frac{\partial c}{\partial \rho}\frac{3}{\rho} - \frac{\partial c}{\partial \rho}\frac{1}{\rho}\\ &= \frac{\partial^2 c}{\partial \rho^2} + \frac{\partial c}{\partial \rho}\frac{2}{\rho} = \frac{1}{\rho^2}\frac{\partial}{\partial \rho}\left(\rho^2\frac{\partial c}{\partial \rho}\right)\end{aligned} \tag{11}$$

(b) Integrating the equation in part (a) with respect to ρ twice, we obtain

$$c = \frac{a_1}{\rho} + a_2 \tag{12}$$

where a_1 and a_2 are constants. The boundary condition that $c(\rho_1,t) = c_1$and $c(\rho_2,t) = c_2$ indicates that $a_1 = \frac{(c_1-c_2)\rho_1\rho_2}{\rho_2-\rho_1}$ and $a_2 = \frac{c_2\rho_2-c_1\rho_1}{\rho_2-\rho_1}$.

8. The characteristic curve is determined by the following system of ODEs

$$\begin{aligned}\frac{dx}{ds} &= x, \quad x(0) = x_0\\ \frac{dt}{ds} &= 1, \quad t(0) = 0\\ \frac{dz}{ds} &= 0, \quad z(0) = \phi(x_0)\end{aligned} \tag{13}$$

where $z(s) = u(x(s),t(s))$. Then

$$x(s) = x_0 e^s, \quad t(s) = s \quad \text{and} \quad z(s) = \phi(x_0) \tag{14}$$

Solving for x_0 and s with respect to x and t and plugging back into $z(s)$, we obtain the solution is

$$u(x,t) = \phi(xe^{-t}). \tag{15}$$

9. Assume that $u(x,y) = X(x)Y(y)$, then $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$ is transformed into

$$\frac{X''(x)}{X(x)} = -\frac{Y''(y)}{Y(y)} \tag{16}$$

Since both sides are functions of different variables but they are equal, they must be constants,say λ, i.e.

$$\frac{X''(x)}{X(x)} = \lambda \quad \text{and} \quad \frac{Y''(y)}{Y(y)} = -\lambda \tag{17}$$

From the boundary condition of $u(x,t)$, the boundary conditions for $X(x)$ are $X(0) = X(L_1) = 0$ and the boundary conditions for $Y(y)$ is $Y(0) = 0$. Based on the theory of Sturm-Liouville problems, a non-trivial solution to X(x) must be of the form

$$X_n(x) = \sin\left(\frac{n\pi x}{L_1}\right) \qquad n = 1, 2, \cdots \tag{18}$$

with $\lambda_n = -\frac{n^2\pi^2}{L_1^2}$. Then, the solution to $Y(y)$ must be

$$Y(y) = a_1 \exp\left(\frac{n\pi}{L_1}y\right) + a_2 \exp\left(-\frac{n\pi}{L_1}y\right) \tag{19}$$

Its boundary condition $Y(0) = 0$ gives that $a_2 = -a_1$. Thus, the solution to $Y(y)$ can be shown as follows by ignoring the constant

$$Y(y) = \exp\left(\frac{n\pi}{L_1}y\right) - \exp\left(-\frac{n\pi}{L_1}y\right) \tag{20}$$

Since we assume that $u(x,y) = X(x)Y(y)$ and by using the principle of superpositions, a solution to $u(x,y)$ can be given as

$$u(x,y) = \sum_{n=1}^{\infty} A_n \left(\exp\left(\frac{n\pi}{L_1}y\right) - \exp\left(-\frac{n\pi}{L_1}y\right)\right) \sin\left(\frac{n\pi x}{L_1}\right) \tag{21}$$

The last boundary condition that $u(x,L_2) = f(x)$ determines that

$$A_n = \frac{2}{\left(\exp\left(\frac{n\pi L_2}{L_1}\right) - \exp\left(-\frac{n\pi L_2}{L_1}\right)\right) L_1} \int_0^{L_1} f(x) \sin\left(\frac{n\pi x}{L_1}\right) dx. \tag{22}$$

10. Let $v(x,t) = e^{ct}u(x,t)$, then

$$\begin{cases} \frac{\partial v}{\partial t} - \frac{\partial^2 v}{\partial x^2} = e^{ct} f(x,t) \\ v(x,0) = g(x) \end{cases} \tag{23}$$

The solution to equation (23) can be obtained as,

$$v(x,t) = \int_{-\infty}^{\infty} g(y)\Phi(x-y,t)dy + \int_0^t \int_{-\infty}^{\infty} e^{cs} f(y,s)\Phi(x-y,t-s)dyds \tag{24}$$

Therefore,

$$u(x,t) = e^{-ct}\left(\int_{-\infty}^{\infty} g(y)\Phi(x-y,t)dy + \int_0^t \int_{-\infty}^{\infty} e^{cs} f(y,s)\Phi(x-y,t-s)dyds\right) \tag{25}$$

11. (a) The exact solution obtained from the method of characteristics is given as follows,

$$u(x,t) = \begin{cases} 1, & x \le t \\ 0, & x > t \end{cases} \tag{26}$$

(b) $v_1^1 - v_1^0 + \frac{\Delta t}{\Delta x}(v_2^0 - v_1^0) = 0$ where, from the initial condition, $v_1^0 = v_2^0 = 0$. Thus, the one-sided scheme gives $v_1^1 = 0$, which is not the correct answer since $u(\Delta x, \Delta t) = 1$ since $\Delta x \le \Delta t$.

References

[1] A. Okubo. *Diffusion and ecological problems: mathematical models*. Springer-Verlag, 1980.

[2] H. Risken. *The Fokker-Plack equation: Methods of solution and application*. Springer-Verlag, 1984.