MATHEMATICAL MODELLING 2013

SOLUTIONS TO EXERCISES 1-3

Exercise 1

Model the following i-level processes as unimolecular or bimolecular reactions:

1. Migration from one habitat to another (unimolecular or monomolecular reaction)

$$A \xrightarrow{\alpha} B. \tag{1}$$

The corresponding differential equations are:

$$\begin{cases} \frac{da(t)}{dt} = -\alpha a(t), \\ \frac{db(t)}{dt} = -\alpha a(t). \end{cases}$$

2. Asexual reproduction

$$A \xrightarrow{\alpha} A + A,$$

with differential equation:

$$\frac{da}{dt} = -\alpha a + 2\alpha a = \alpha a.$$

Note that the $+2\alpha a$ comes from the fact that we have twice the product from the left. It is the reactant on the left that determines the speed of the process not the resulting products. It will be clear in the next example, see equation (3).

3. Territory owner starts a fight with an intruder (formation of a bound state)

$$A + B \xrightarrow{\alpha} F, \tag{2}$$

with differential equations:

$$\begin{cases} \frac{da}{dt} = -\alpha ab, \\ \frac{db}{dt} = -\alpha ab, \\ \frac{df}{dt} = \alpha ab. \end{cases} \tag{3}$$

Remark that $\frac{df}{dt} = \alpha ab$ and not $\cancel{\alpha f}$.

4. Hatching of an egg

$$A \xrightarrow{\alpha} B.$$

This example is similar to example 1, equation (1) in which the subject changes state.

5. Predator captures prey

$$A + B \xrightarrow{\alpha} F.$$

This example is similar to example 3, equation (2) where there is formation of a bound.

6. Death

$$A \xrightarrow{\alpha} \emptyset \text{ or if you prefer } A \xrightarrow{\alpha} \dagger.$$

The associated differential equation is

$$\frac{da}{dt} = -\alpha a.$$

7. Sexual reproduction

This problem can be viewed in various ways which don't give the same differential equations.

- First, we can consider the original particle as a couple.

$$A \xrightarrow{\alpha} A + B,$$

where A can be considered as a bound state of two particles (Father+Mother). With differential equations:

$$\begin{cases} \frac{da}{dt} = -\alpha a + \alpha a = 0, \\ \frac{db}{dt} = \alpha a. \end{cases}$$

- It can also be viewed as two independent particles meeting.

$$F + M \xrightarrow{\alpha} F + M + B,$$

then the differential equations are:

$$\begin{cases} \frac{df}{dt} = -\alpha fm + \alpha fm = 0, \\ \frac{dm}{dt} = -\alpha fm + \alpha fm = 0, \\ \frac{db}{dt} = \alpha fm. \end{cases}$$

Note that the differential equations for $\frac{db}{dt}$ are not the same.

8. Predator discovers prey and starts stalking the prey

$$A + B \xrightarrow{\alpha} S,$$

even if you consider that the prey didn't realize that the predator is after her/him, it is part of a predator-prey complex. The differential equations are:

$$\begin{cases} \frac{da}{dt} = -\alpha ab, \\ \frac{db}{dt} = -\alpha ab, \\ \frac{ds}{dt} = \alpha ab. \end{cases}$$

9. Two competitors meet and one eliminates the other

$$A + A \xrightarrow{\alpha} A + \dagger,$$

with differential equations:

$$\frac{da}{dt} = -\alpha a^2 + \frac{1}{2}\alpha a^2 = -\frac{\alpha}{2}a^2,$$

Exercise 2

We consider the following reactions

$$A \xrightarrow{\alpha} B \tag{4}$$

and

$$2A \xrightarrow{\alpha} A + B \tag{5}$$

1. What i-level could they represent?

   For (4), it represents single particle changing state independently of any other particle.

   - egg hatching
   - migration from one place to another
   - maturation
   - recovery from illness

   For (5), you need interaction of two similar i-states to modify one of them

   - interference competition

2. For each reaction, solve the corresponding differential equations for the concentration of A.

   Let $a(t)$ denote the concentration of A which we will write in short a.

   In the case (4), the differential equation is

   $$\frac{da}{dt} = -\alpha a,$$

   which has as a solution

   $$a(t) = e^{-\alpha(t-t_0)} a(t_0). \tag{6}$$

   If we choose the origin time $t_0 = 0$ then equation (6) simplifies to $a(t) = a(0)e^{-\alpha t}$ where $a(0)$ is the initial condition.

   In the case (5), the differential equation is

   $$\frac{da}{dt} = -\alpha a^2 + \frac{1}{2}\alpha a^2 = -\frac{1}{2}\alpha a^2,$$

   which has as a solution

   $$a(t) = \frac{a(t_0)}{1 + \frac{\alpha a(t_0)(t-t_0)}{2}}.$$

   Let $t_0 = 0$ then $a(t) = \frac{a(0)}{1+\frac{1}{2}\alpha a(0)t}$.

3. Let T be the time when a particular A-particle undergoes a reaction counting from $t = 0$. For each reaction, give the probability density of T and calculate its expected value.

   Let $F(t)$ denote the distribution function of T also called cumulative distribution function of T and let $f(t)$ denote the probability density function of T.

   $F(t)$ is an increasing function continuous on the right with limit on the left (cadlag) which verifies

   $$\lim_{t \to -\infty} F(t) = 0 \qquad \lim_{t \to +\infty} F(t) = 1$$

   and is defined by $\mathbb{P}\{T \leq t\} = F(t)$. If $F(t)$ is differentiable then

   $$F'(t) = f(t). \tag{7}$$

Therefore

$$\mathbb{P}\{T \leq t\} = F(t) = \int_{-\infty}^{t} f(u)du.$$

By definition of the distribution function

$$F(t) = \mathbb{P}\{T \leq t\} = 1 - \mathbb{P}\{T > t\}.$$

By the Strong Law of Large Numbers (SLLN) $\mathbb{P}\{T > t\}$ =fraction of particles A still present at time t is $\frac{a(t)}{a(0)}$. Therefore

$$\begin{aligned} F(t) &= 1 - \mathbb{P}\{T > t\}, \\ &= 1 - \frac{a(t)}{a(0)}. \end{aligned} \tag{8}$$

(a) In the case (4), then the equation (8) turns into

$$F(t) = 1 - \frac{a(t)}{a(0)}, \tag{9}$$

$$= 1 - e^{-\alpha t}. \tag{10}$$

Using (7), we find

$$f(t) = F'(t) = \alpha e^{-\alpha t}$$

and the expectation is

$$\begin{aligned} \mathbb{E}(T) &= \int_0^\infty t f(t) dt, \\ &= \int_0^\infty \alpha t e^{-\alpha t} dt. \end{aligned}$$

By integration by parts with

$$\begin{aligned} u &= t & u' &= 1 \\ v' &= \alpha e^{-\alpha t} & v &= -e^{-\alpha t} \end{aligned}$$

we get

$$\begin{aligned} \mathbb{E}(T) &= \left[-te^{-\alpha t}\right]_0^\infty + \int_0^\infty e^{-\alpha t} dt, \\ &= \left[-te^{-\alpha t}\right]_0^\infty - \left[\frac{1}{\alpha} e^{-\alpha t}\right]_0^\infty, \\ &= \frac{1}{\alpha}. \end{aligned}$$

Remark that the expected waiting time decreases with the intensity α.

(b) In the case (5), then the equation (8) turns into

$$F(t) = 1 - \frac{a(t)}{a(0)}, \tag{11}$$

$$= 1 - \frac{1}{1 + \frac{1}{2}\alpha a(0) t}. \tag{12}$$

Using (7), we find

$$f(t) = F'(t) = \frac{\frac{1}{2}\alpha a(0)}{\left(1 + \frac{1}{2}\alpha a(0) t\right)^2}$$

and the expectation is

$$\mathbb{E}(T) = \int_0^\infty tf(t)dt,$$
$$= \int_0^\infty \frac{1}{2}\alpha a(0)\frac{t}{\left(1+\frac{1}{2}\alpha a(0)t\right)^2}dt.$$

Let $c = \frac{1}{2}\alpha a(0)$ to simplify the notations then

$$\mathbb{E}(T) = \int_0^\infty \frac{ct}{(1+ct)^2}dt,$$

where $\frac{ct}{(1+ct)^2} = \frac{1}{1+ct} - \frac{1}{(1+ct)^2}$. Therefore

$$\begin{aligned}\mathbb{E}(T) &= \int_0^\infty \frac{1}{1+ct} - \frac{1}{(1+ct)^2}dt,\\ &= \int_0^\infty \frac{1}{1+ct}dt - \int_0^\infty \frac{1}{(1+ct)^2}dt,\\ &= [\log(1+ct)]_0^\infty + \left[\frac{1}{c}\frac{1}{1+ct}\right]_0^\infty,\\ &= +\infty.\end{aligned}$$

(c) Determination of the reaction constant α

- In the case (4) then $a(t) = a(0)e^{-\alpha t}$ so

$$\log a(t) = \log a(0) - \alpha t.$$

Hence, if we draw $\log a$ with respect to t then the coordinate at the origin is $\log a(0)$ and the slope is $-\alpha$.

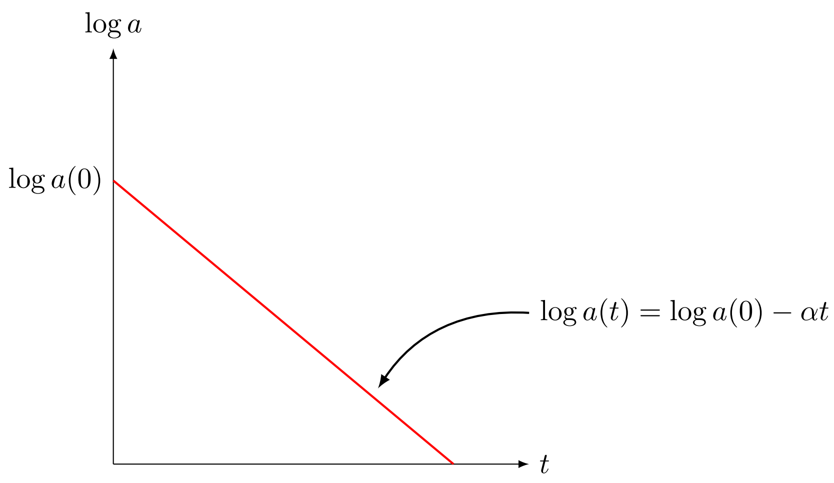

Figure 1: Determining the reaction constant in the case $A \xrightarrow{\alpha} B$.

- In the case (5) then $a(t) = \frac{a(0)}{1+\frac{1}{2}\alpha a(0)t}$ so

$$\begin{aligned}\frac{1}{a} &= \frac{1+\frac{1}{2}\alpha a(0)t}{a(0)},\\ &= \frac{1}{2}\alpha t + \frac{1}{a(0)}.\end{aligned}$$

Hence, if we draw $\frac{1}{a}$ with respect to t then the coordinate at the origin is $\frac{1}{a(0)}$ and the slope is $\frac{1}{2}\alpha$.

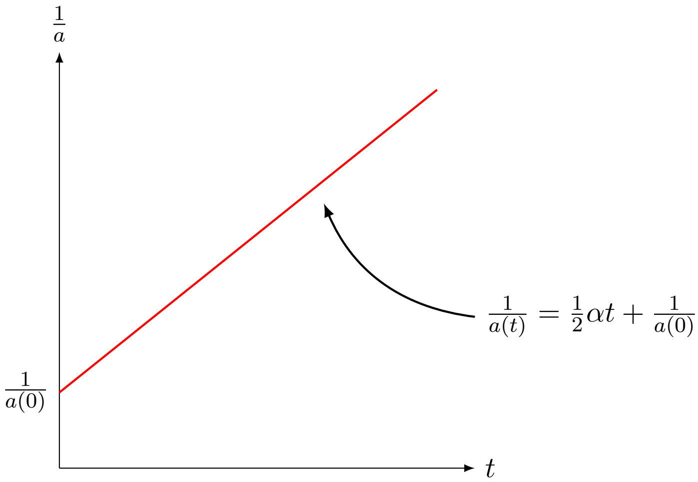

Figure 2: Determining the reaction constant in the case $A + A \xrightarrow{\alpha} A + B$.

Exercise 3

Let E denote an egg, A an adult and R an adult recodering from egg laying, and consider the following reaction network:

$$\begin{array}{rcr}
\text{egg hatching:} & E \xrightarrow{\alpha} B & (1) \\
\text{reproduction:} & A \xrightarrow{\beta} R + E & (2) \\
\text{recovery:} & R \xrightarrow{\gamma} A & (3) \\
\text{cannibalism:} & E + A \xrightarrow{\delta} A & (4) \\
\text{death of egg:} & E \xrightarrow{\lambda} \dagger & (5) \\
\text{death of } A\text{-adult:} & A \xrightarrow{\alpha} \dagger & (6) \\
\text{death of } R\text{-adult:} & R \xrightarrow{\alpha} \dagger & (7)
\end{array}$$

Give the corresponding differential equations for the population densities of eggs, adults and adults in the recovery phase.

$$\begin{array}{ccccccccc}
 & & (1) & (2) & (3) & (4) & (5) & (6) & (7) \\
\frac{de}{dt} & = & -\alpha e & +\beta a & & -\delta ea & -\lambda e & & \\
\frac{da}{dt} & = & \alpha e & -\beta a & +\gamma r & & & -\mu a & \\
\frac{dr}{dt} & = & & \beta a & -\gamma r & & & & -\nu r
\end{array}$$