Math 2E03- Introduction to Modelling

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The law of mass action The rate of increase in product or decrease in reactant may be referred to simply as the rate of the reaction, denoted by R. The law of mass action states that the rate of a chemical reaction is proportional to the product of the concentration of the reactions. For instance the reaction

$$A + B \rightarrow^{k} P \tag{1}$$

We have the follwoing reaction rate R

$$R = k[A][B] \tag{2}$$

We may write the reaction rate in three ways. Let's assume $a = [A], b = [B]$ and $p = [P]$

(3)
$$\frac{da}{dt} = -kab$$
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$$\frac{dp}{dt} = kab$$

Conservation law: The sum of the rate of change of the concentrations of any one of the product species and any one of the reactant species remains constant throughout a constant volume reaction.

$$\dot{a} + \dot{p} = 0$$
$$\dot{b} + \dot{p} = 0 \tag{6}$$

Physically, this means that loss of reactant results in a gain in product and that no matter may be lost or gained in the process. From the equation (5)

$$\frac{d(a-b)}{dt} = 0$$
$$\frac{d(a+p)}{dt} = 0 \quad (7)$$
$$\frac{d(b+p)}{dt} = 0$$

So $a = b + a_0 - b_0$, $a = p_0 + a_0 - p$ and $b = p_0 + b_0 - p$ which may substitute in to equation (5)

$$\frac{da}{dt} = -ka(a - a_0 + b_0) \quad (8)$$
$$\frac{db}{dt} = -kb(b + a_0 - b_0, \frac{dp}{dt} = k(p_0 + a_0 - p)(p_0 + b_0 - p)$$

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$$\dot{a} = \dot{b} = -k_1 ab + k_{-1} c$$
$$\dot{c} = k_1 ab - k_{-1} c - k_2 c \quad (10)$$
$$\dot{d} = \dot{e} = k_2 c$$

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$$\begin{aligned} \dot{a} = \dot{b} &= -k_1 ab + k_{-1} c \\ \dot{c} &= k_1 ab - k_{-1} c - k_2 c \\ \dot{d} = \dot{e} &= k_2 c \end{aligned} \tag{11}$$

Here also conservation law holds: $\dot{a} + \dot{c} + \dot{d} = 0$

Population type models

No one exists within a vaccum. We all interact with others in some manner, whether benefical or not.To truly capture the essence of the population of a certain species in a particular geographical area, one must take in to account the predator and prey present to hunt/nourish the species. We thus look at ODEs that not only take into account a positive (or negative) effects of the species population itself, but also at the postive or negative effects of interactions with other species.

What is main difference between epidemic type and population type models?.

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What is main difference between epidemic type and population type models?.
In epidemic type models we have a fixed tottal number of individuals but this is not the case with population type models. Now we allow for creation and no longer count dead or lost individuals.

The standard Predator/Prey Model

The standard predator prey model is as follows (we use the example of foxes for the predators and rabbits for the prey)

$$\dot{x} = (-a + by)x \ (x = \text{ predator})$$
$$\dot{y} = (c - dx)y \ (y = \text{ prey}) \tag{12}$$

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- $-ax$ This is natural death rate of predator. This might at first not make sense, as we usually associate a natural birth rate with animals. For example like rabbits (as in the prey ODE) this is true, But with large predators like foxes, lions, etc. the greater the population the greater the tendency for them to die out faster than they are born. They only survive by finding prey to eat, whereas prey typically have abundant food and can flourish.

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Stability analysis:

Let's look for the point of equilibrium

$$\begin{aligned} \dot{x} &= (-a+by)x = 0 \implies x = 0 \text{ or when } y = \frac{a}{b} \\ \dot{y} &= (c-dx)y = 0 \implies y = 0 \text{ or when } x = \frac{c}{d} \end{aligned} \tag{17}$$

We now introduce perturbations to our euilibrium points to determine their stability- we will start with $(\frac{c}{d}, \frac{a}{b})$. We will add perturbations that are functions of time ($\epsilon(t)$ and $\delta(t)$) to the equilibrium points as before and see whether they diminsh to zero (for stable points), grow with time (for unstable point).

$$
\begin{aligned}
x &= \frac{c}{d} + \epsilon \\
y &= \frac{a}{b} + \delta \\
\dot{x} &= (\frac{c}{d} + \epsilon)^{\cdot} \\
\dot{y} &= (\frac{a}{b} + \delta)^{\cdot}
\end{aligned} \tag{18}
$$

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$$\dot{\epsilon} = [-a + b(\frac{a}{b} + \delta)](\frac{c}{d} + \epsilon)$$

$$\dot{\epsilon} = \frac{bc}{d}\delta + b\epsilon\delta \quad (21)$$

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Similarly

$$\dot{\delta} = -\frac{ad}{b}\epsilon$$

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\dot{\epsilon} &= \frac{bc}{d}\delta
\end{aligned} \tag{23}
$$

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We can also solve this system of ODEs directly.

$$
\begin{aligned}
\dot{\epsilon} &= \frac{bc}{d}\delta \\
\dot{\delta} &= -\frac{ad}{b}\epsilon
\end{aligned} \tag{24}
$$