MATH 448 — Week 6

Reaction networks and mass action kinetics

Every model this semester has been built by reasoning through the biology from scratch each time. Reaction networks give a single recipe that writes down the differential equations directly, once the underlying events are listed — and, as a check on the recipe itself, it should be able to reproduce every model already built.

Terms

- **Species**: the quantities being tracked (e.g. X, Y, or S, I, R).
- **Reaction**: an event converting some species into others, written *reactants* $\to$ *products*, with a **rate constant**.
- **Mass action kinetics**: the rate of a reaction is its rate constant times the product of its reactant concentrations. Each species' rate of change is the sum, over every reaction it appears in, of $(\pm 1) \times$ (that reaction's rate) — negative where the species is a reactant, positive where it is a product.

Problem 6.1. Find the ODE for the reaction $X \to 2X$ with rate constant k.

Solution. The rate of this reaction is $k \cdot [X] = kx$. Each time it occurs, one X is consumed and two are produced, a net gain of one X. So

$$\frac{dx}{dt} = kx,$$

exponential growth — the very first model of the semester, recovered from a single reaction.

Lotka–Volterra as a reaction network. Three events: prey reproduce, predators consume prey, predators die.

Predator–prey

$$X \to 2X \text{ (rate } \alpha), \qquad X + Y \to 2Y \text{ (rate } \beta), \qquad Y \to \varnothing \text{ (rate } \gamma).$$

Problem 6.2. Find the mass-action ODEs for this network.

Solution. The three reaction rates are αx, βxy, γy. X is a reactant only in the second reaction; Y is a product of the second and a reactant of the third:

$$\frac{dx}{dt} = \alpha x - \beta xy, \qquad \frac{dy}{dt} = \beta xy - \gamma y.$$

This is exactly the Lotka–Volterra model from Lecture 9, with $\delta = \beta$: one predator is produced for every prey consumed. The general model, with an independent conversion efficiency δ, needs a fourth reaction ($X + Y \to X + 2Y$, prey acting as a catalyst for predator reproduction) alongside $X + Y \to Y$ in place of $X + Y \to 2Y$; the single-reaction version above is the special case where consumption and conversion are the same event.

Epidemics. Two events: a susceptible person meets an infected one and catches the disease; an infected person recovers.

SIR

$$S + I \to 2I \text{ (rate } \beta), \qquad I \to R \text{ (rate } \gamma).$$

Problem 6.3. Find the mass-action ODEs for the SIR network, and find the condition on the total population $N = S + I + R$ under which an infection introduced into an otherwise healthy population ($S \approx N$, I small) actually grows.

Solution. The two rates are βsi and γi:

$$\frac{ds}{dt} = -\beta si, \qquad \frac{di}{dt} = \beta si - \gamma i, \qquad \frac{dr}{dt} = \gamma i.$$

Near the start, $s \approx N$, so $di/dt \approx i(\beta N - \gamma)$. This is positive — the infection grows — exactly when

$$R_0 := \frac{\beta N}{\gamma} > 1.$$

R_0, the *basic reproduction number*, is the single threshold that decides whether an outbreak happens at all.

SIS. If recovery gives no lasting immunity (replace $I \to R$ with $I \to S$), the same bookkeeping gives

$$\frac{ds}{dt} = -\beta si + \gamma i, \qquad \frac{di}{dt} = \beta si - \gamma i,$$

with $s + i = N$ fixed. Setting $i = 0$ with $s = N - i$ gives $i = 0$ or $i = N - \gamma/\beta$: a positive *endemic* equilibrium exists exactly when $R_0 = \beta N/\gamma > 1$ — the same threshold as SIR, now marking permanent disease persistence instead of a one-time outbreak.

MATLAB: simulating a reaction network

```
be=0.3; ga=0.1; N=1000; % change these to explore R0
f = @(t,z) [-be*z(1)*z(2); be*z(1)*z(2)-ga*z(2); ga*z(2)];
[t,Z] = ode45(f, [0 160], [N-1; 1; 0]);
plot(t,Z(:,1), t,Z(:,2), t,Z(:,3))
legend('S','I','R'); xlabel('t')
```

Scenario: malaria. Malaria is not transmitted person to person — it needs a mosquito in between. In small groups, propose the species and reactions for a population of humans and a population of mosquitoes, where a human infects a mosquito and a mosquito infects a human.

Problem 6.4. Write down a reaction network for malaria, treating both recovery (humans only) and infection as separate events, and find the resulting ODEs.

Solution. Let S_h, I_h be susceptible and infected humans, S_m, I_m susceptible and infected mosquitoes.

$$S_h + I_m \to I_h + I_m \ (\beta_h), \qquad S_m + I_h \to I_m + I_h \ (\beta_m), \qquad I_h \to S_h \ (\gamma).$$

The first reaction lets an infected mosquito convert a human without being consumed itself (a catalyst); likewise the second for an infected human converting a mosquito. Mass action gives

$$\dot{S}_h = -\beta_h S_h I_m + \gamma I_h, \quad \dot{I}_h = \beta_h S_h I_m - \gamma I_h, \quad \dot{S}_m = -\beta_m S_m I_h, \quad \dot{I}_m = \beta_m S_m I_h.$$

Unlike Lotka–Volterra's conserved quantity H (Lecture 9), the conservation law here is elementary: no reaction creates or destroys a human or a mosquito, only converts infection status, so $S_h + I_h$ and $S_m + I_m$ are each exactly constant — visible directly from the network, without needing to find or verify anything.

Scenario: zombies.[1] A susceptible person bitten by a zombie becomes a zombie; zombies are occasionally destroyed by survivors. Propose the species and reactions.

Problem 6.5. Write down a reaction network for a zombie outbreak and find the resulting ODEs. What do you notice?

Solution. With S, Z, R (susceptible, zombie, permanently removed):

$$S + Z \to 2Z \text{ (rate } \beta), \qquad Z \to R \text{ (rate } \delta).$$

$$\dot{S} = -\beta SZ, \qquad \dot{Z} = \beta SZ - \delta Z, \qquad \dot{R} = \delta Z.$$

[1] P. Munz, I. Hudea, J. Imad, R. J. Smith?, "When Zombies Attack!: Mathematical Modelling of an Outbreak of Zombie Infection," in *Infectious Disease Modelling Research Progress*, Nova Science, 2009, pp. 133–150. (The model below is a simplified version for a first exposure; their actual paper adds a latent period, quarantine, and more.)

This is the SIR network again, with Z playing the role of I: the same threshold applies, $\beta N/\delta > 1$ for the outbreak to take off, where $N = S + Z + R$. A wildly different story, identical mathematics.

Exercise 6.1. Add a third event to the SIR network: a recovered person loses immunity and becomes susceptible again, at rate μ (an "SIRS" model). Find the resulting ODEs.

Exercise 6.2. (*computer exploration*) Using the MATLAB code above (adjusted for the malaria or zombie network), find, by trial and error, the threshold value of β (holding the other parameters fixed) below which an initial handful of infected individuals dies out rather than spreading.