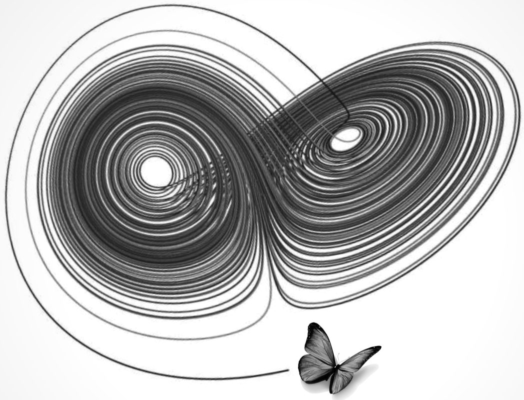
Biology and Dynamical Systems



Week 4: Simplifying models and starting simulations

Today's aim is to show what we can do to visualize our equations so we can think about them concretely

Outline:

Why you do we simplify our models?

Reducing variables and equations

Running Simple Simulations

Why we have to simplify our models (before we start plugging away at simulations)

We really can't keep more than a handful of things in our head at once

7 7 3 2 6 3 0 1 8 1
vs
(773) 263-0181

Every free parameter in a model means you have to do **exponentially** more simulation and analysis

5 params vs 6 params

x^5 x^6

No one wants to look at a totally disorganized mess of equations

$$\frac{dc}{dt} = \frac{k_1}{k_2}c + k_{ph}c - k_r c + \frac{K^2}{k_b T}$$

vs

$$\frac{dc}{dt} = k_{on} - k_{off}c$$

There are really 3 parts to a model

$$\frac{dc}{dt} = k_{on} - k_{off}c$$

Variables: the values (like concentration) that are changing,

a,b,c,x,y,z

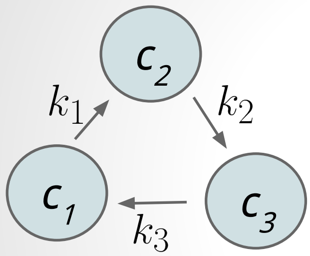
Parameters: the constants that define the system

k_on, k_off, D, α

The form of the equation: where do the variables show up in the equation

___dc/dt = ___ - ___c

The most important simplification is definitely limiting the number of variables/equations



cyclical reaction

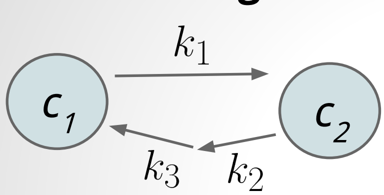
$$c_1 + c_2 + c_3 = C$$

$$\frac{dc_1}{dt} = k_3 c_3 - k_1 c_1$$

$$\frac{dc_2}{dt} = k_1 c_1 - k_2 c_2$$

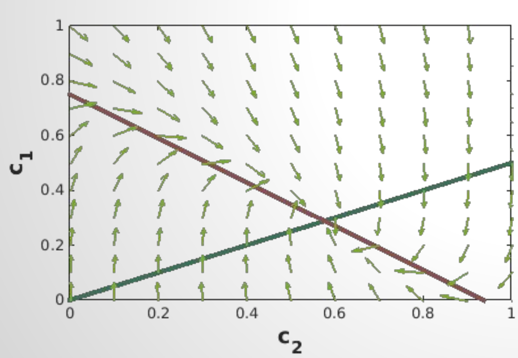
$$\frac{dc_3}{dt} = k_2 c_2 - k_3 c_3$$

The equation got slightly more complicated, but now we no longer have to worry about c_3 at all



$$\frac{dc_1}{dt} = k_3 C - k_3 c_2 - (k_3 + k_1) c_1$$

$$\frac{dc_2}{dt} = k_1 c_1 - k_2 c_2$$



$$c_1^* = \frac{k_3 C}{k_1 + k_3} - \frac{k_3 c_2^*}{k_1 + k_3}$$

$$c_1^* = \frac{k_2 c_2^*}{k_1}$$

We can use a numerical differential equation solver to simulate the output of a simplified system

$$\frac{dc_1}{dt} = k_3 C - k_3 c_2 - (k_3 + k_1) c_1 \qquad \frac{dc_2}{dt} = k_1 c_1 - k_2 c_2$$

we must pick explicit values for each of our constants in the equations

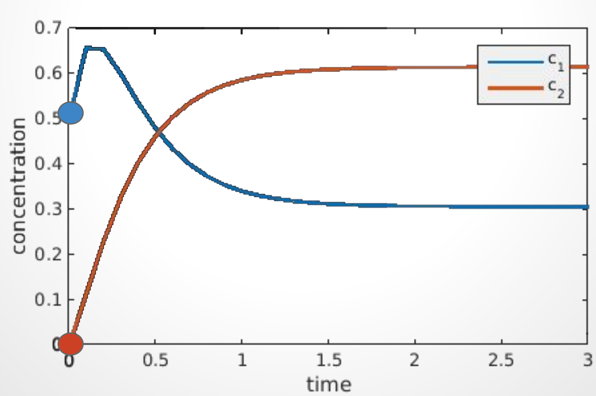
$$\frac{dc_1}{dt} = 1 * 8 - 8 * c_2 - (2 + 8) * c_1 \qquad \frac{dc_2}{dt} = 2 * c_1 - 1 * c_2$$

we must pick explicit starting values for both c_1 and c_2

$$c_1 = 0.5 \qquad c_2 = 0$$

The computer simulates by simply following the "protocol" over lots and lots of small steps

$$\frac{dc_1}{dt} = 1 * 8 - 8 * c_2 - (2 + 8) * c_1 \qquad \frac{dc_2}{dt} = 2 * c_1 - 1 * c_2$$



In MATLAB, all we have to do is define the equation and then set our variables and initial conditions

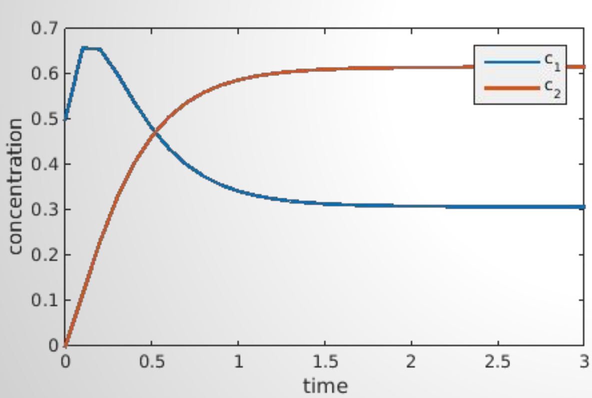
$$\frac{dc_1}{dt} = k_3C - k_3c_2 - (k_3 + k_1)c_1$$
$$\frac{dc_2}{dt} = k_1c_1 - k_2c_2$$

```
function dc = myode(t,c,C,k1,k2,k3)
        c1 = c(1);
        c2 = c(2);
        dc1 = k3*C - k3*c2 - (k3+k1)*c1;
        dc2 = k1*c1 - k2*c2;
        dc = [dc1;dc2];
end
```

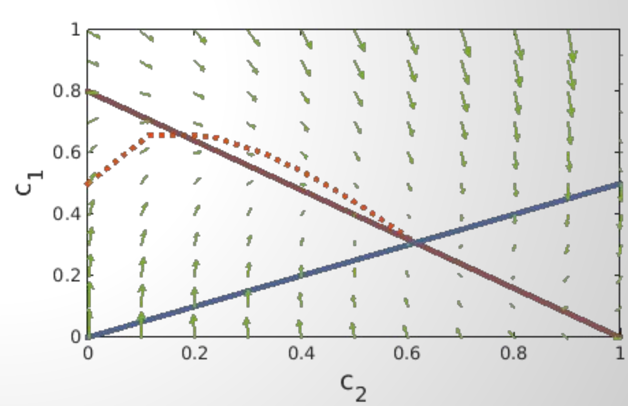
```
t = 0:0.1:10;
c0 = [1,0];

C = 1; k1=2; k2=1; k3=8;

[t, c] = ode45(@myode,t,c0,[],C,k1,k2,k3);
```

We can plot the output as "concentrations vs time" or on top of the nullcline and arrows as "c_1 vs c_2"

plot(t,c(:,1),t,c(:,2))



plot(c(:,2),c(:,1))



Discussion: Let's do some simple simulations (40 pts)

1. Break into groups
2. Each group will get a differential equation with a description of a system
3. Work for a few minutes to implement the simulations
   a. First convert the 3 component system into 2 components (5 pts)
   b. Change the sample code to implement the new equation (5 pts)
   c. Plot both types of output graphs (10 pts)
4. We'll regroup after 15-20 minutes and go through each one
5. 10 pts for explaining your reasoning
6. 10 pts for giving good feedback to others

Project: Simplify and graph your system

1. Continue with the system you wrote about in the last project assignment
2. Try to simplify your equations again (5 pts)
   a. Try to use tricks like the ones we came up with today
3. Pick constant values and initial conditions that makes sense (5 pts)
4. Simulate your simplified system and graph the outputs (10pts)
5. Change the constants and document how the output changes (10 pts)
6. Explain what your simulation taught you about your system (10 pts)
   a. How did the behavior depend on your choice of constants

Reading: Read the one-page handout and be ready for a simple quiz at the start of next week

1. There will be a 5 minute, 4 question (10 pts each) quiz at the start of next class.
2. It is just designed to determine if you read the handout.
3. You probably won't even have to think if you do the reading.