Calculating Biological Quantities CSCI 2897

Prof. Daniel Larremore Lecture 2

daniel.larremore@colorado.edu @danlarremore

Lecture 2 Plan

1. One minute review of the basics:

- 1. Website
- 2. Syllabus
- 3. Canvas
- 4. Slack
- 2. Office Hours?
- 3. Asking "modeling" questions
- 4. Some vocabulary
- 5. Steps to modeling a biological problem (1-4)

Last Time on CBQ...

- Website: https://github.com/dblarremore/CSCI2897
 - Homework & reading posted, Code examples, Class notes
- Syllabus: https://github.com/dblarremore/CSCI2897#syllabus
- Canvas: Turn in homework, Check grades
- Slack: Didn't get the invite? Stick around after class—we'll get you set up!
- Textbook: See Slack.

First assignment already posted on Canvas — due Tuesday. [Easy!]

The Quiz

Universe	Votes		
Star Wars 🗙	6 (4)	Thornton Colorado Springs (2) Durango Fort Collins Highlands Ranch	Normal, IL Dearborn, MI Austin, TX San Francisco, CA Fremont, CA
Star Trek 🗸	2 (4)		
Marvel X	2		
IDK 🗙	1	Wheat Ridge	,

[&]quot;Boring AF"

[&]quot;Suburbia Hell but in the middle of nowhere"

[&]quot;Really fun because I love the outdoors"

[&]quot;Great!"

[&]quot;Hot, but alright"

[&]quot;A very nice place with world class mountain biking."

[&]quot;Surfing & traveling"

[&]quot;Got a bit boring by the time I was 16"

[&]quot;I am going to be brutally honest — it's kinda boring.

Dynamical Models 101: Ask a question

- Think about a problem that puzzles you.
- Draw a diagram that illustrates the various processes at work.
- Dynamical models describe how a system changes over time.

Models, Vocab, and 7 Steps

Deterministic vs Stochastic dynamical models

Deterministic models assume that the future is entirely predicted (i.e. determined) by the model.

• Stochastic models assume that random (stochastic) events affect the system.

1. Formulate the question

- 1. Formulate the question
- 2. Determine the basic ingredients

- 1. Formulate the question
- 2. Determine the basic ingredients
- 3. Qualitatively describe the biological system

- 1. Formulate the question
- 2. Determine the basic ingredients
- 3. Qualitatively describe the biological system
- 4. Quantitatively describe the biological system

- 1. Formulate the question
- 2. Determine the basic ingredients
- 3. Qualitatively describe the biological system
- 4. Quantitatively describe the biological system
- 5. Analyze the equations

- 1. Formulate the question
- 2. Determine the basic ingredients
- 3. Qualitatively describe the biological system
- 4. Quantitatively describe the biological system
- 5. Analyze the equations
- 6. Checks & balances

- 1. Formulate the question
- 2. Determine the basic ingredients
- 3. Qualitatively describe the biological system
- 4. Quantitatively describe the biological system
- 5. Analyze the equations
- 6. Checks & balances
- 7. Relate the results back to the question

1. Formulate the question

2. Determine the basic ingredients

- Variables: what entities might change over time?
- Assign a letter to each variable. (Hint: use "intuitive" letters!)
- Write down fundamental constraints on your variables.
- Write down reasonable constraints on your variables.

Discrete time vs Continuous time

Discrete time models:

Continuous time models:

• Note:

Be clear about your time scale

- Time scale: the unit of time between t=0 and t=1.
 - How much time is in the *tick of the clock?*
- Discrete time models:

Continuous time models:

btw...

- You'll have to decide whether your variables are discrete or continuous too!
 - Often, discrete values get **SO BIG** that you can model a discretized population using a continuous variable.

Sometimes, you can reinterpret a discrete variable in continuous units.

Why might we do this?

Equations!

Recursion Equations

- A recursion equation describes the value of a variable in the next time step.
 - n(t+1) = "some function of n(t)"
- Examples.

Difference Equations

 A difference equation describes the difference between a variable's values in two successive time steps

$$\Delta n = n(t+1) - n(t) =$$
 "some function of $n(t)$ "

• Examples.

Differential Equations

• A differential equation describes the rate of change of the variable over time

$$\frac{dn(t)}{dt} = \text{"some function of } n(t)\text{"}$$

• Examples.

Intuition?

Suppose that
$$\frac{dn(t)}{dt} = 0$$

(A) Sketch the derivative
$$\frac{dn(t)}{dt}$$
 vs. $n(t)$.

(B) Sketch the variable n(t) vs time.

Suppose that
$$\frac{dn(t)}{dt} = 1$$

(A) Sketch the derivative
$$\frac{dn(t)}{dt}$$
 vs. $n(t)$.

(B) Sketch the variable n(t) vs time.

Suppose that
$$\frac{dn(t)}{dt} = -k$$

(A) Sketch the derivative
$$\frac{dn(t)}{dt}$$
 vs. $n(t)$. (B) Sketch the variable $n(t)$ vs time.

Suppose that
$$\frac{dn(t)}{dt} = \sqrt{n(t)}$$

(A) Sketch the derivative
$$\frac{dn(t)}{dt}$$
 vs. $n(t)$.

(B) Sketch the variable n(t) vs time.

Parameters

- The **parameters** of the model are quantities that influence the dynamics but remain fixed over time.
- Examples:

Parameters

- The **parameters** of the model are quantities that influence the dynamics but remain fixed over time.
- When we fix parameters and look at a trajectory of the equation, that's called forward simulation or forward integration. Model + Parameters → Data
- When we have data and a model, and we determine the values of the parameters that best fit the data, that's parameter inference. Model + Data → Parameters

- Note: parameters' units need to match the kind of model we're using.
- Note: parameters may have reasonable ranges in addition to fundamental ranges.

- 1. Formulate the question
- 2. Determine the basic ingredients
- 3. Qualitatively describe the biological system
- 4. Quantitatively describe the biological system
- 5. Analyze the equations
- 6. Checks & balances
- 7. Relate the results back to the question

Diagrams: Life Cycle

• Keep track of the events occurring during a single time step and their order.

Diagrams: Flow

• Keep track of the events occurring during a single time step and their order.

Diagrams: Table of Events

• Discrete-time models with multiple events per time step and multiple variables.

Pros and Cons?

• See Otto & Day, Chapter 2.4

- 1. Formulate the question
- 2. Determine the basic ingredients
- 3. Qualitatively describe the biological system
- 4. Quantitatively describe the biological system
- 5. Analyze the equations
- 6. Checks & balances
- 7. Relate the results back to the question

Example: tree branching

• Use the life cycle diagram to derive a recursion, and use that to create a difference equation.

Example: mouse model

• Use the life cycle diagram to derive the stages of the recursion.

Recipes: recursion & difference equations from life cycle diagrams

- 1. Use n'(t), n''(t), n'''(t) etc to denote the variable's value after each life cycle event.
- 2. Set n(t + 1) to the value of n after the final event in the cycle.
- 3. Substitute, and get n(t + 1) in terms of n(t) by eliminating n'(t) etc.
- 4. [Bonus] Subtract n(t) from both sides and simplify to get the difference equation $\Delta n = n(t+1) n(t) = \dots$

Example: COVID-19

• Use the flow diagram to create the recursion equations for COVID-19 spread.

Recipes: differential equations from flow diagrams

$$\frac{d(n(t))}{dt} = \dots$$

the flow rates along arrows entering the circle

- + the flow rates along arrows leaving & returning to the circle
- the flow rates along arrows exiting the circle

- 1. Formulate the question
- 2. Determine the basic ingredients
- 3. Qualitatively describe the biological system
- 4. Quantitatively describe the biological system
- 5. Analyze the equations
- 6. Checks & balances
- 7. Relate the results back to the question