CS 346 –
Computational Modeling & Simulation I
(Interdisciplinary Science)

Professor Eric Aaron

Lecture – T R 11:00am

Lecture Meeting Location: It’s complicated…

Lab Meeting Location: It’s complicated…

Business

• Reading: Ch. 2.2-2.3 in the textbook

• HW1 out now, due Mar. 10 (see assignment sheet for details)
  – This is phase 1 of a 2-phase assignment
  – Please submit work on time, so we can move on to the next phase (see assignment sheet for lateness policy)

• In general in CS346, please treat given deadlines as firm / exact
  – They’re the same for everybody
  – … But if you’d like an extension, let me know, and we’ll see about giving an extension to everybody!

And if there are extenuating circumstances (e.g., illness, personal crisis), please let me know!
Business, pt. 2

- Please contact me if your Lab0 isn’t yet checked off
  - It’d be great to get everyone’s lab done by the end of this week

- Reading assignment: Webb’s *Can robots make good models of biological behaviour?*
  - Available via Colby’s library; see link from CS346 *Useful Links and Additional Notes*
  - A *small assignment* asking you to read this paper and write short responses (a few sentences) to two questions is posted on course HWs page
  - Due by end of day Friday, Mar. 5 (but, lateness penalties will be delayed… I’ll email about that)

But What If The Growth / Decay Function Is More Complicated Than That?

- When possible, analytic solutions are good for differential equations, but some functions don’t have analytic solutions
- Systems too complex for analytic solutions can be analyzed by modeling and simulation!
  - I.e., instead of solving the relationship analytically, can approximate it using numerical methods
  - Simulation involves computing values based on time advancing in small steps (approximating the infinitesimal used in the derivative)

- *Finite difference equation:* Approximates using a derivative
  \[
  \text{population}(t) = \text{population}(t-\Delta t) + (\text{popn RateOfChange} * \Delta t)
  \]
  - Gives a *numerical approximation* to the derivative (i.e., rate of change)
  - Repeat this with advancing values of \( t \) to see pop’n growth over time
Main Idea: Simulation and Approximation to an Unknown Function

- Consider the problem of calculating the shape of an unknown curve which starts at a given point and satisfies a given differential equation
  - For this application, a differential equation can be thought of as a formula by which the slope of the tangent line to the curve can be computed at any point on the curve, once the position of that point has been calculated
- The curve is initially unknown
- Starting point \( A_0 \) is known
- Procedure:
  - From the differential equation, compute slope of the curve at \( A_0 \) (and therefore, the tangent line)
  - Take a small step along that tangent line to point \( A_1 \)
  - Pretend that \( A_1 \) is still on the curve
  - Apply same procedure as for point \( A_0 \) above
- After several steps, a polygonal curve is computed
- *Error between the two curves will be small if step size is small enough and interval of computation is finite*

Approximating Unconstrained Growth

initialize \( \text{simulationLength} \)
initialize \( \text{population} \)
initialize \( \text{irog} \) %-growth constant
initialize \( \Delta t \)

\[
\text{numIterations} \leftarrow \frac{\text{simulationLength}}{\Delta t}
\]

for \( i = 1 : \text{numIterations} \) do

\[
\text{popn\_GrowthRate} \leftarrow \text{irog} \times \text{population}
\]

\[
\text{Δpopulation} \leftarrow \text{popn\_GrowthRate} \times \Delta t
\]

\[
\text{population} \leftarrow \text{population} + \Delta \text{population}
\]

\[
t \leftarrow i \times \Delta t
\]

display \( t, \text{population} \)

(Also display \( \Delta \text{population} \) or \( \text{popn\_GrowthRate} \), if desired)
A Model Example

- In a lab, 100 bacteria were put in a culture to grow
- How do we model this? What process should we follow?
A Model Example

• In a lab, 100 bacteria were put in a culture to grow
• How do we model this? What process should we follow?
  – Assumptions: Lab environment, so we’ll assume ample food, nothing to kill the bacteria—*unconstrained growth*
  – Variables needed: P₀ (initial population), r (intrinsic rate of growth)
  – Differential equation: \( \frac{dP}{dt} = rP \)
  – Analytic solution: \( P = P₀ \cdot e^{rt} \)
• Let’s see what it looks like when graphed in Matlab
  – Assume \( r = 0.1 \)
  – We’ll try three graphs; in all, time \( t = 1:\text{<some_interval>}:50 \)
  – Three test intervals: 0.01, 0.001, 0.0001
  – How do the three resulting graphs / functions differ from each other?

A Model Example with Finite Difference Equations

• In a lab, 100 bacteria were put in a culture to grow
• How do we model this?
  – \( P₀ = 100; \ r = 0.1; \ P = P₀ \cdot e^{rt} \)
• How would we simulate this with difference equations?
  – With \( \Delta t = 0.5 \), is it a good match to the analytic solution? How about \( \Delta t = 1 \)?
  – How does changing \( r \) affect how good a match the simulated difference equation is to the analytic solution?
  – (What tests do you want to do to find out?)
initialize simulationLength
initialize population
initialize irog % growth constant
initialize $\Delta t$

$numIterations \leftarrow \text{simulationLength} / \Delta t$

for $i = 1 : numIterations$ do
    $\text{popn\_GrowthRate} \leftarrow irog \times \text{population}$
    $\Delta \text{population} \leftarrow \text{popn\_GrowthRate} \times \Delta t$
    $\text{population} \leftarrow \text{population} + \Delta \text{population}$
    $t \leftarrow i \times \Delta t$
    display $t$, population

(Also display $\Delta \text{population}$ or $\text{popn\_GrowthRate}$, if desired)

Some Matlab Code for Generating Plots

```matlab
% test 1: sampling at interval 0.01
interval = 0.01; % sampling interval for graphing
t = 0:interval:50; % array of times for plotting on x axis
q = p0 * exp(irog*t); % unconstrained growth function
plot(t,q);
legend(sprintf('Analytic solution: \%d*exp(%g*t); interval %g', ...
    p0, irog, interval));

% test 2: sampling at interval 0.001
interval2 = 0.001; % sampling interval for test 2
figure;
t2 = 0:interval2:50; % array of times for test 2
q2 = p0 * exp(irog*t2);
plot(t2,q2);
The code continues, of course...
```
Some Matlab Code for Generating Plots

% test 1: sampling at interval 0.01
interval = 0.01; % sampling interval for graphing
t = 0:interval:50; % array of times for plotting on x axis
q = p0 * exp(irog*t); % unconstrained growth function
plot(t,q);
legend(sprintf('Analytic solution: %d*exp(%g*t); interval %g', p0,irog,interval));

% test 2: sampling at interval 0.001
interval2 = 0.001; % sampling interval for test 2
figure;
t2 = 0:interval2:50; % array of times for test 2
q2 = p0 * exp(irog*t2);
plot(t2,q2);

The code continues, of course...

Constrained Growth

- Is the unconstrained growth model a good one for natural organisms in natural environments?
  - Probably not. Limited resources, etc., can constrain growth
- Vocab: The carrying capacity $M$ for an organism in an environment is the maximum population size of that organism supported by that environment.
  - E.g., if a deer refuge can support at most 1000 deer, we say $M$ for the deer in the refuge is 1000.

Notation question for programmers and computer scientists: In the example, $M$ is used to represent carrying capacity. What do you think of that notation?

- How to revise our unconstrained growth model to incorporate M?

$$\frac{dP}{dt} = rP$$

$$P = P_0 e^{rt}$$
Constrained Growth

- How to revise our unconstrained growth model to incorporate $M$?
- Desired behavior of the revised model
  - When population far less than $M$, growth should be similar to unconstrained model
  - When population near $M$, growth should be nearly 0 (births nearly equal deaths)

- So, how could we incorporate $M$ in the model?
  - What approaches might we consider?
  - What variables might we add to the model?
  - One suggestion: Let’s say we have the number of births represented as $rP$ for population size $P$ and growth constant $r$...
  - … we could have a number of deaths also represented. What might be the equation specifying the rate of change of number of deaths?

\[
\frac{dP}{dt} = rP
\]

\[
P = P_0 e^{rt}
\]
Constrained Growth

- How to revise our unconstrained growth model to incorporate M?
- Desired behavior of the revised model
  - When population far less than M, growth should be similar to unconstrained model
  - When population near M, growth should be nearly 0 (births nearly equal deaths)
- So, how could we incorporate M in the model?
- The number of births is represented as $rP$. For the number of deaths (call it $D$), the rate of change should fit certain constraints
  - When population size P is much less than M, the death rate should be very low
    - Asymptotically, we might think that when P nears 0, the death rate should near 0
  - When P is nearly M, the death rate should be nearly equal to the birth rate
    - Asymptotically, we might think that when P gets to M, the death rate gets equal to the birth rate
- What is a candidate model (equation) that has this behavior?

\[
\frac{dP}{dt} = rP \\
P = P_0 e^{rt}
\]