Calculating Biological Quantities

CSCI 2897

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Lecture 2

Lecture 2 Plan

1. **One minute review of the basics:**
    1. Website
    2. Syllabus
    3. Canvas
    4. Slack
2. ~~**Office Hours?**~~ Survey!
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)
Star Trek ✅	2 (4)
Marvel ❌	2
IDK ❌	1

Thornton
Colorado Springs (2)
Durango
Fort Collins
Highlands Ranch
Wheat Ridge

Normal, IL
Dearborn, MI
Austin, TX
San Francisco, CA
Fremont, CA

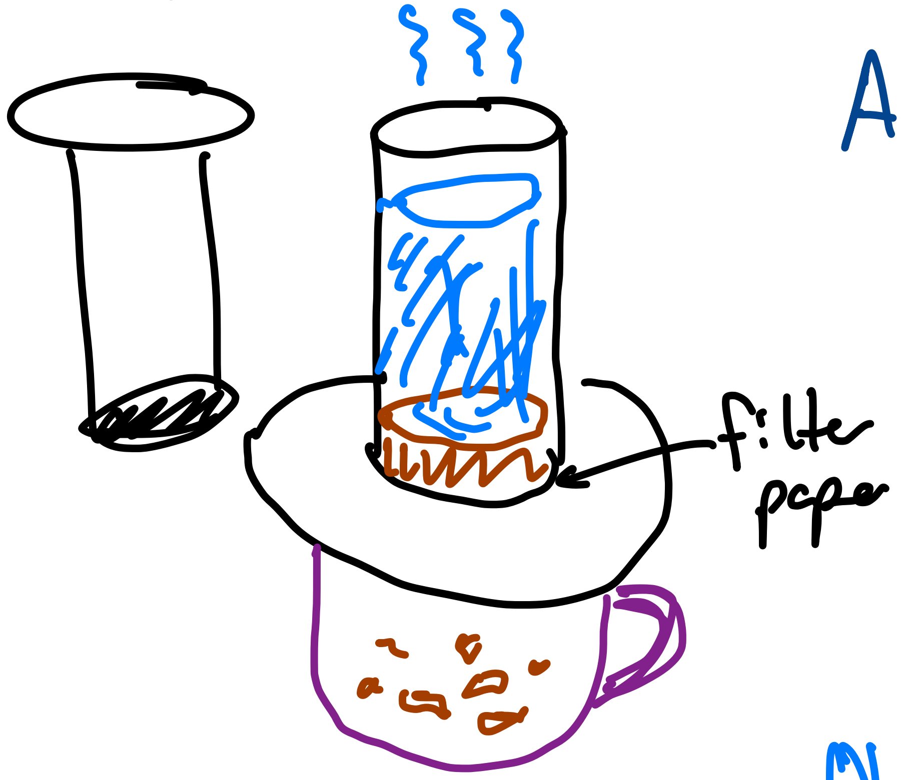
"Boring AF"
"Suburbia Hell but in the middle of nowhere"
"Really fun because I love the outdoors"
"Great!"
"Hot, but alright"

"A very nice place with world class mountain biking."
"Surfing & traveling"
"Got a bit boring by the time I was 16"
"I am going to be brutally honest — it's kinda boring.

Dynamical Models 101: Ask a question

Idea: How long is the line for handouts at the Be Involved Fair?

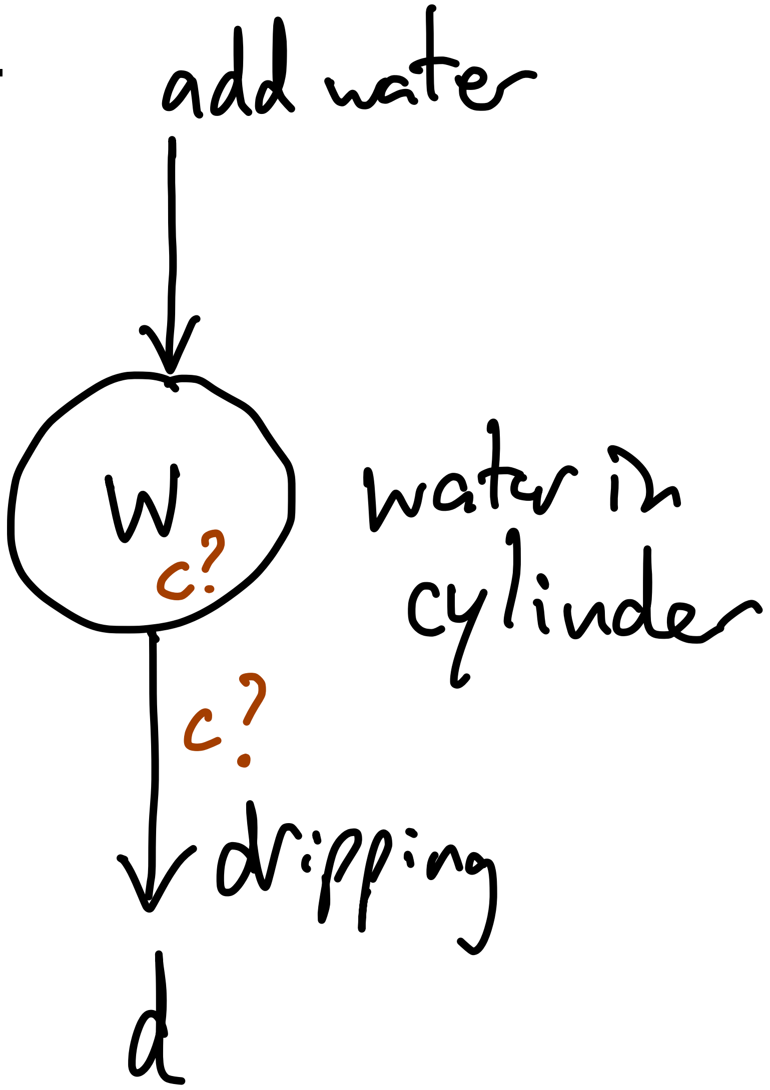
- Think about a problem that puzzles you.
- Draw a diagram that illustrates the various processes at work.
- *Dynamical* models describe how a system changes over time.



Aeropress (coffee)

What determines the drip rate into the cup?

Obs: • If I fill to top → dripping
• If I fill halfway → no dripping



variables: 1 dripping
2 water level

parameter: 3 coffee level, c 4 coffee coarseness, x

Models, Vocab, and 7 Steps

Deterministic vs Stochastic dynamical models

this course

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

Q: how much coffee drips from coffee maker?

Model: flow in, flow out

Because there are no random elements → deterministic

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

Q: how much snow is at Eldora?

Model: stochastic snowfall events, stochastic temperature

Because we have stochastic elements → stochastic model

Otto & Day: 7 steps to modeling a biological problem

1. Formulate the question

- what do you want to know?
- describe that in the form of a specific question.
- Boil the question down → as clear and as well-specified as possible.
- Start w/ simplest, biologically reasonable description of the system.

story.

ELI5 – Explain it like I'm five.

Otto & Day: 7 steps to modeling a biological problem

1. Formulate the question
2. Determine the basic ingredients

Define: variables

① constraints. height, $h \geq 0$

② interactions between variables.

Decide: time

discrete. Clear clock ticks. Update rules like Excel.

continuous. ask for values of variables at any time.

time scale how much time passes between $t=0$ and $t=1$? (e.g. a day? seconds? minutes?) units of t.

Define: parameters

- constraints. ① fundamental $0 \leq c \leq 100\%$
  ② reasonable $0 \leq c \leq 25\%$

Otto & Day: 7 steps to modeling a biological problem

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

- Life cycle diagram
- Flow diagram
- Event table

Otto & Day: 7 steps to modeling a biological problem

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

Diagrams (guide) → equations

Checks: • Do our constraints hold?
• Do the units LHS = units RHS?

Big: Can this model help us answer question in step 1?

Otto & Day: 7 steps to modeling a biological problem

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
    - solve (analytical)
    - simulate (numerical)
    - analysis/reasoning

APPM Diff. Eq.

MATH

Otto & Day: 7 steps to modeling a biological problem

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

- check analysis / solution against known examples or data.
- generalizability.
- reflect: alternatives to this model? revisit earlier steps?

Otto & Day: 7 steps to modeling a biological problem

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

- Did your model help you answer the question?
- Intuitive? Counter-intuitive?
- Insights? Tell a story to explain?
- Experiment? Field study?

1. Formulate the question

1. How does # branches on a tree change over time? pop. growth

2. How does having a cat change the # of mice in a field? immigration predation

3. How does # of ppl w/ COVID-19 change over a month? interactions between variables (infectious disease)

Obs: you can tell what the variable is.

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.

\# branches $n(t) \geq 0$

\# mice $m(t) \geq 0$

\# susceptible $S(t) \geq 0$

\# infected/ious $I(t) \geq 0$

\# recovered $R(t) \geq 0$

$S(t) + I(t) + R(t) =$ total population size

notes

- $n(t)$ "of t" reminder that this is a variable.
- Alternatives $n(t)$ "of t"
  n_t "sub t"
  n
- conventions
  n - population
  p - proportion
  $n_1(t)$ - pop 1
  $n_2(t)$ - pop 2

Discrete time vs Continuous time

- **Discrete time models**: "jumpy"
  - assuming that all the modeled actions take place in Δt a single time step
  - ↑ holds well when Δt is v small / reasonable
- **Continuous time models**: "smooth"
  - assume that a variable can change at any point in time, not just between Δt time steps.
  - seems better, but could be unrealistic, depending on process we're modeling. ex: budget.
- **Note:**

Might be easier to work with one type vs the other! (math)

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**:

COVID-19 ~ day

Yeast ~ seconds, minutes

Soil moisture ~ minutes

Climate ~ years, decades

- **Continuous time models**:

Ask: how much time has passed between $t=0$ and $t=1$? units?

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.

      1. individuals → biomass (kg)
      2. individuals → proportions of population.

    - Sometimes, you can reinterpret a discrete variable in continuous units.
    - Why might we do this?

- math is easier!
- code is easier?

$n(t)$	integer	branches
$m(t)$	integer	mice
S, I, R	integer	people

Equations!

Recursion Equations

- A **recursion equation** describes the value of a variable in the next time step.

$$n(t+1) = \text{"some function of } n(t)\text{"}$$

- Examples.

$$\underbrace{n(t+1) = n(t) + n(t-1)}_{\text{looks back two steps = "second order"}}$$

Fibonacci

$n(0) = 6$

$n(1) = 12$

$n(2) = n(1) + n(0)$

$= 12 + 6$

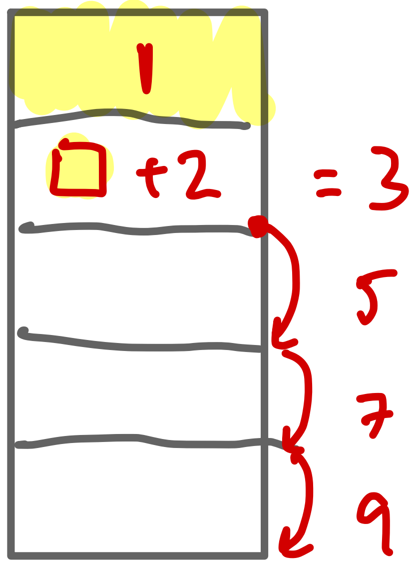
$= 18$

$n(3) = n(2) + n(1)$

$= 18 + 12$

$= 30$

Excel



looks back one step

"first order"

$$n(row+1) = n(row) + 2$$

Exponential Growth:

$$n(t+1) = n(t) \cdot 2$$

Difference Equations

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

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

- Examples.

Excel: $n(t+1) = n(t) + 2$

subtract $n(t)$ from LHS, RHS

$$n(t+1) - n(t) = \cancel{n(t)} + 2 - \cancel{n(t)}$$

$$\boxed{\Delta n = 2}$$

Expon. Growth:

$$n(t+1) = 2n(t)$$

subtract $n(t)$ from LHS RHS

$$n(t+1) - n(t) = 2n(t) - n(t)$$

$$\boxed{\Delta n = n(t)}$$

Differential Equations

- A **differential equation** describes the rate of change of the variable over time

"slope" "derivative"

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

- Examples.

Bank Interest:

$$\frac{dn}{dt} = rn$$

$$\frac{dn(t)}{dt} = r\,n(t)$$

parameter, interest rate

Newton's Law of Cooling

$$\frac{dT}{dt} = -k\left(T(t) - T_{room}\right)$$

param. rate constant

room temp.

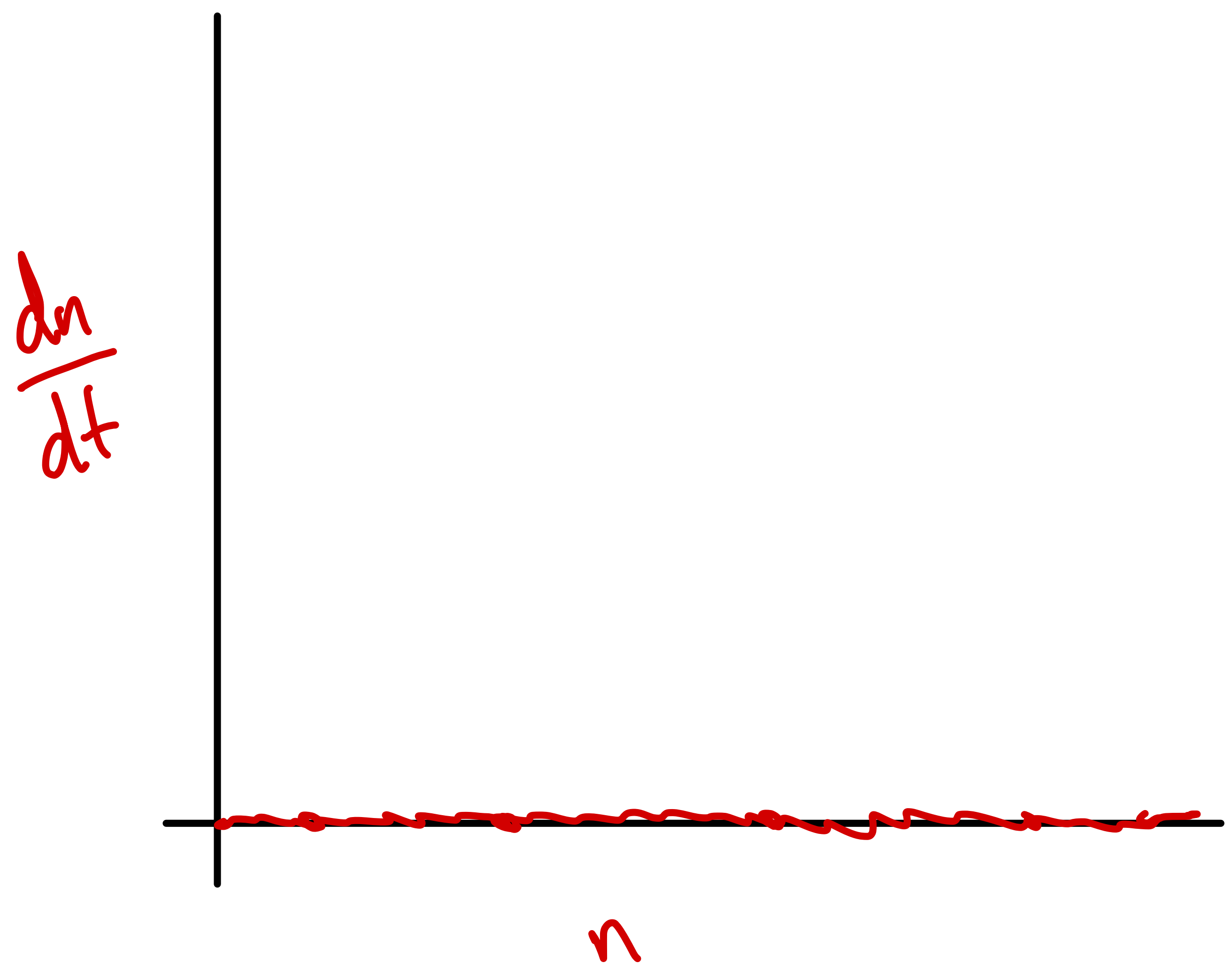
Intuition?

Example 1

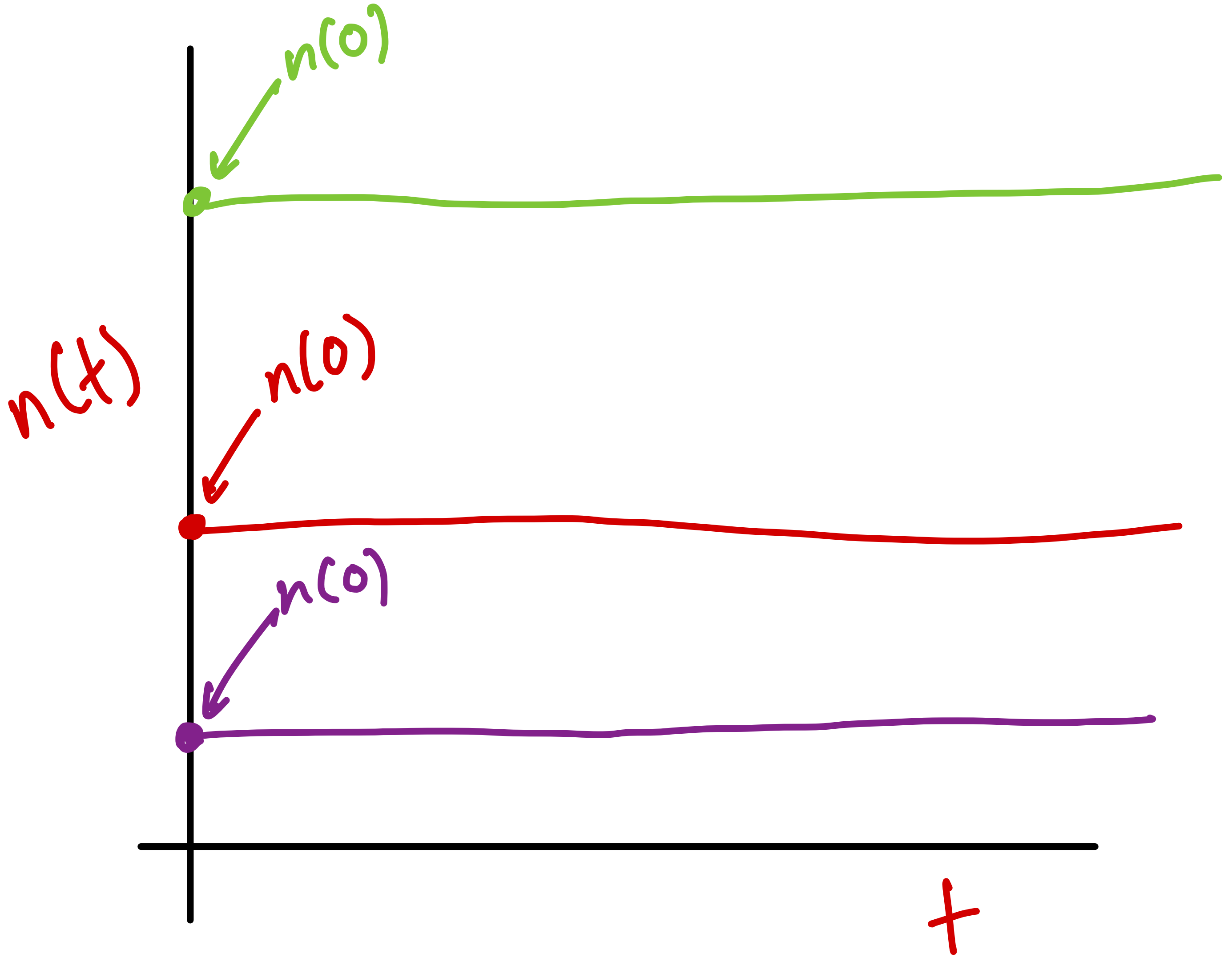
Suppose that $\dfrac{dn(t)}{dt} = 0$

rate of change of n over time = 0 ⇒ n isn't changing

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



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

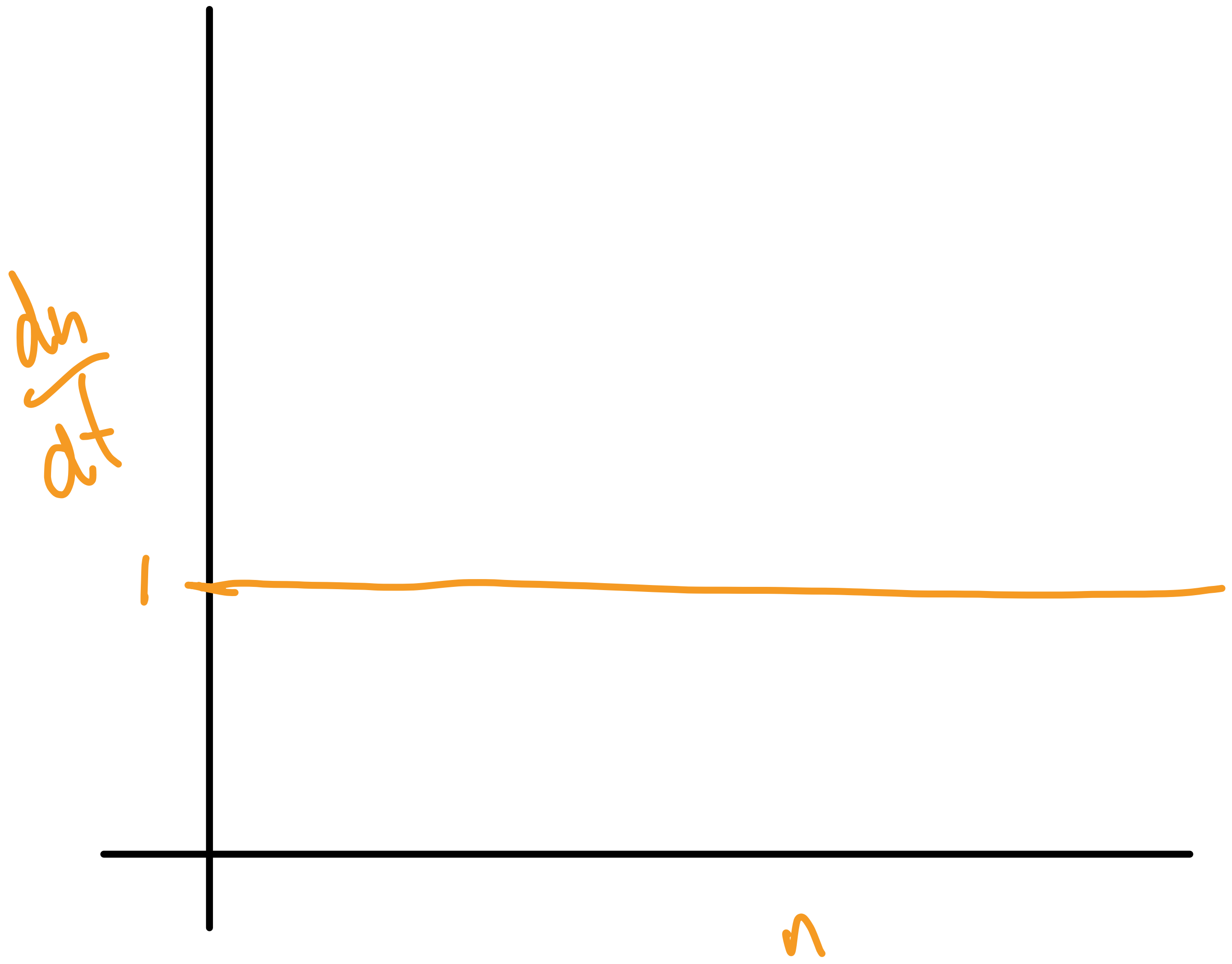


Example 2

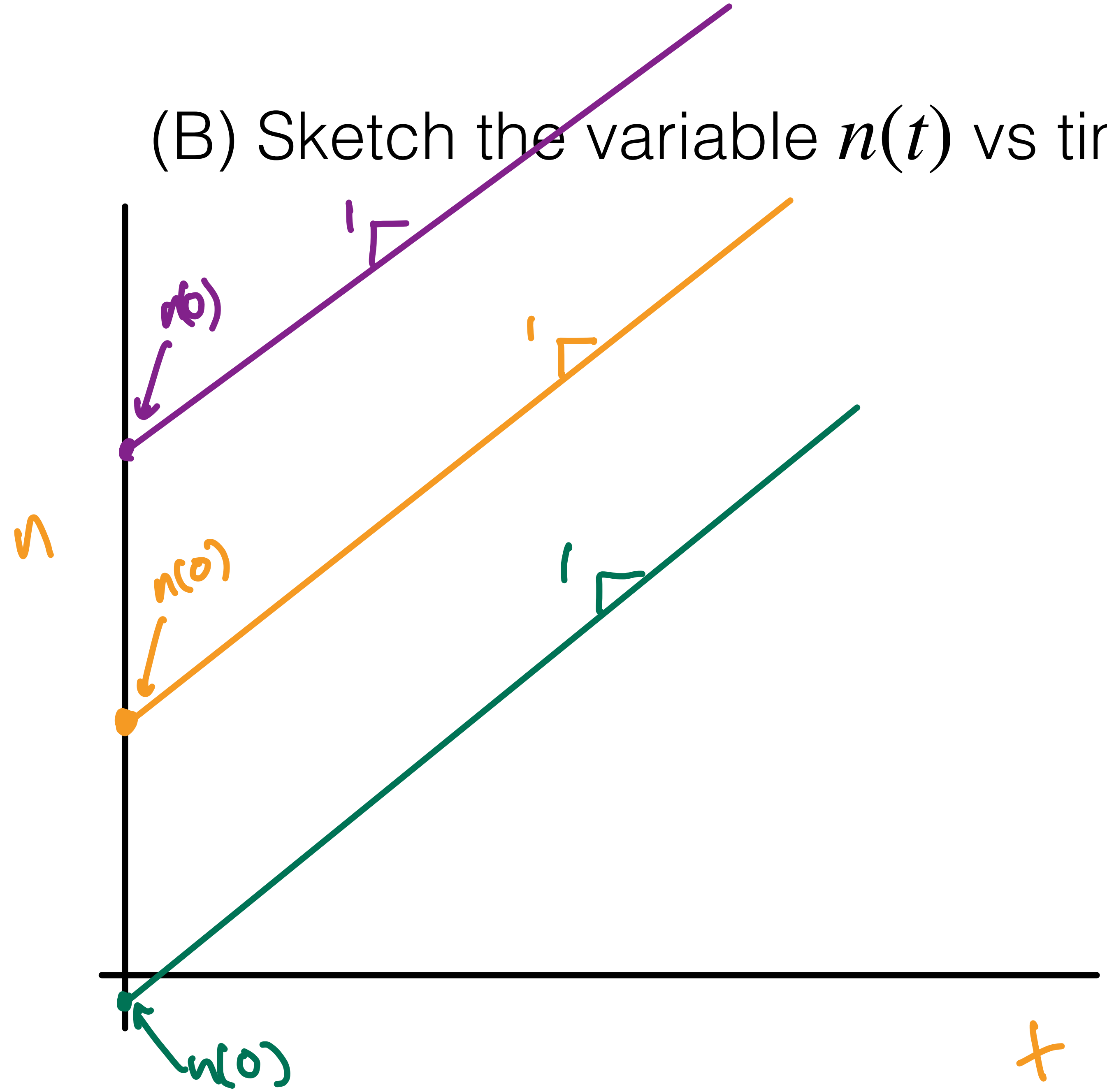
Suppose that $\dfrac{dn(t)}{dt} = 1$

$\frac{dn}{dt}$ is always one.

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



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

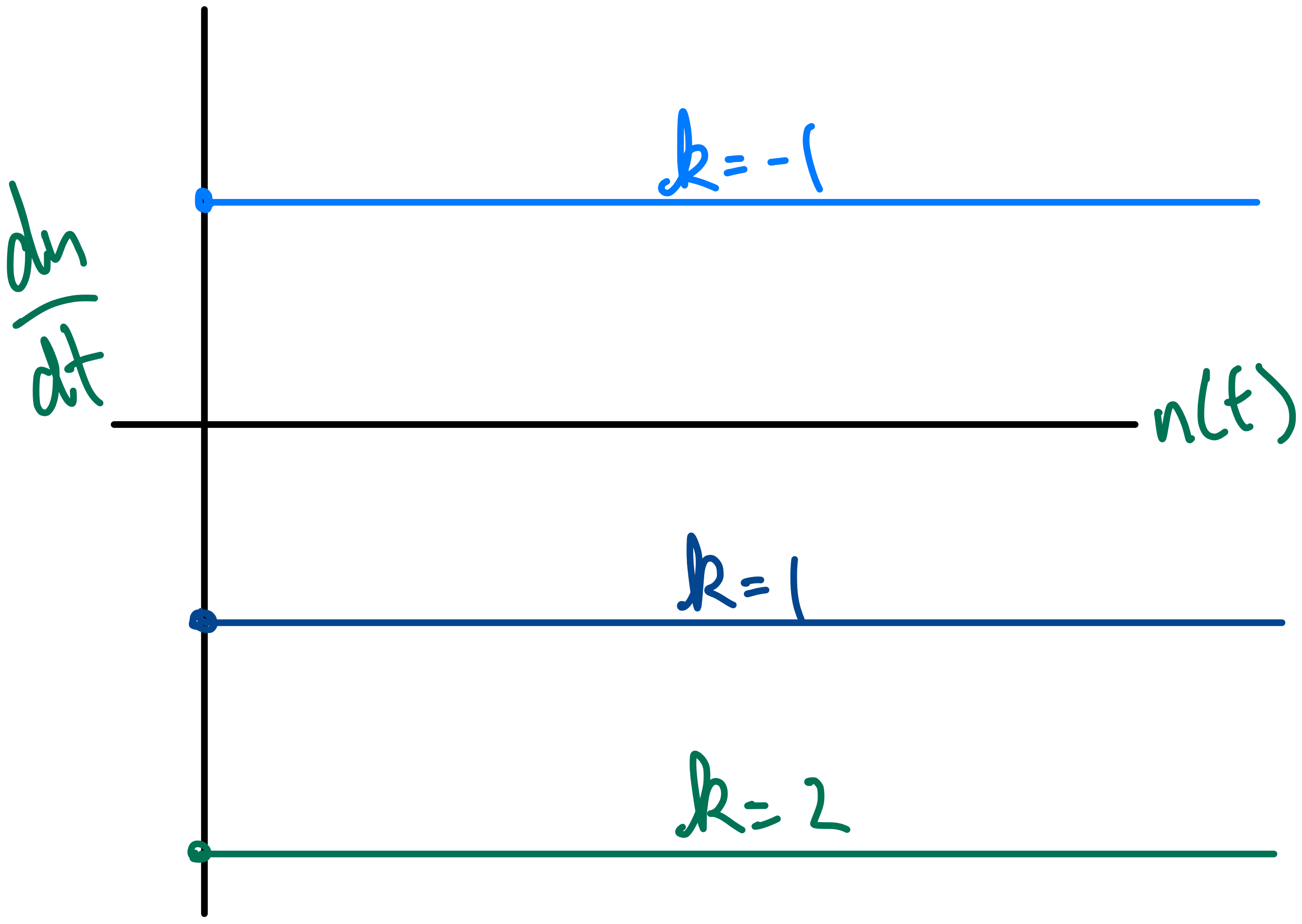


Example 3

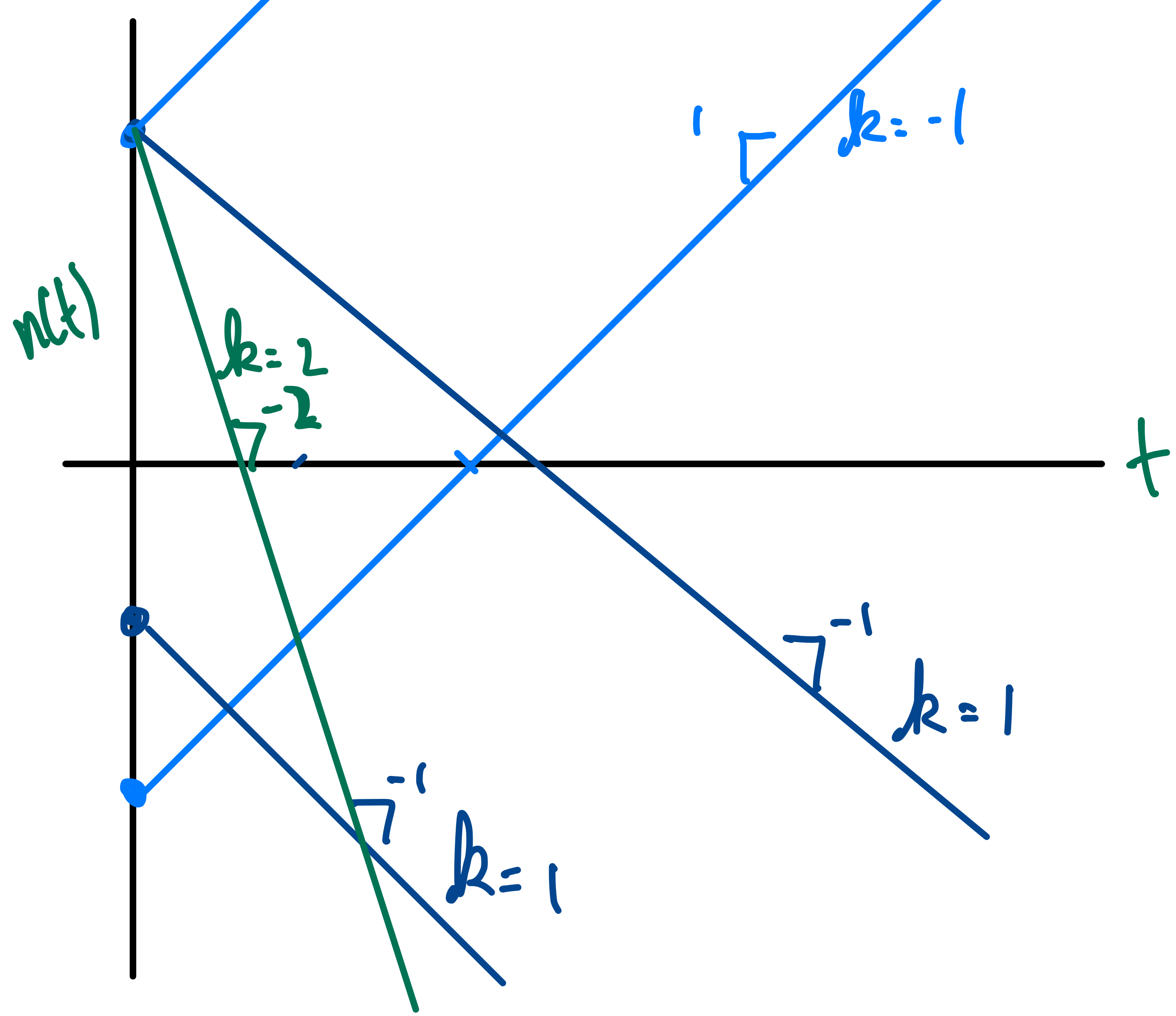
Observation:
- parameters matter
- initial conditions matter ($n(0)$)

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

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



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



Example 4

$y = \sqrt{x}$

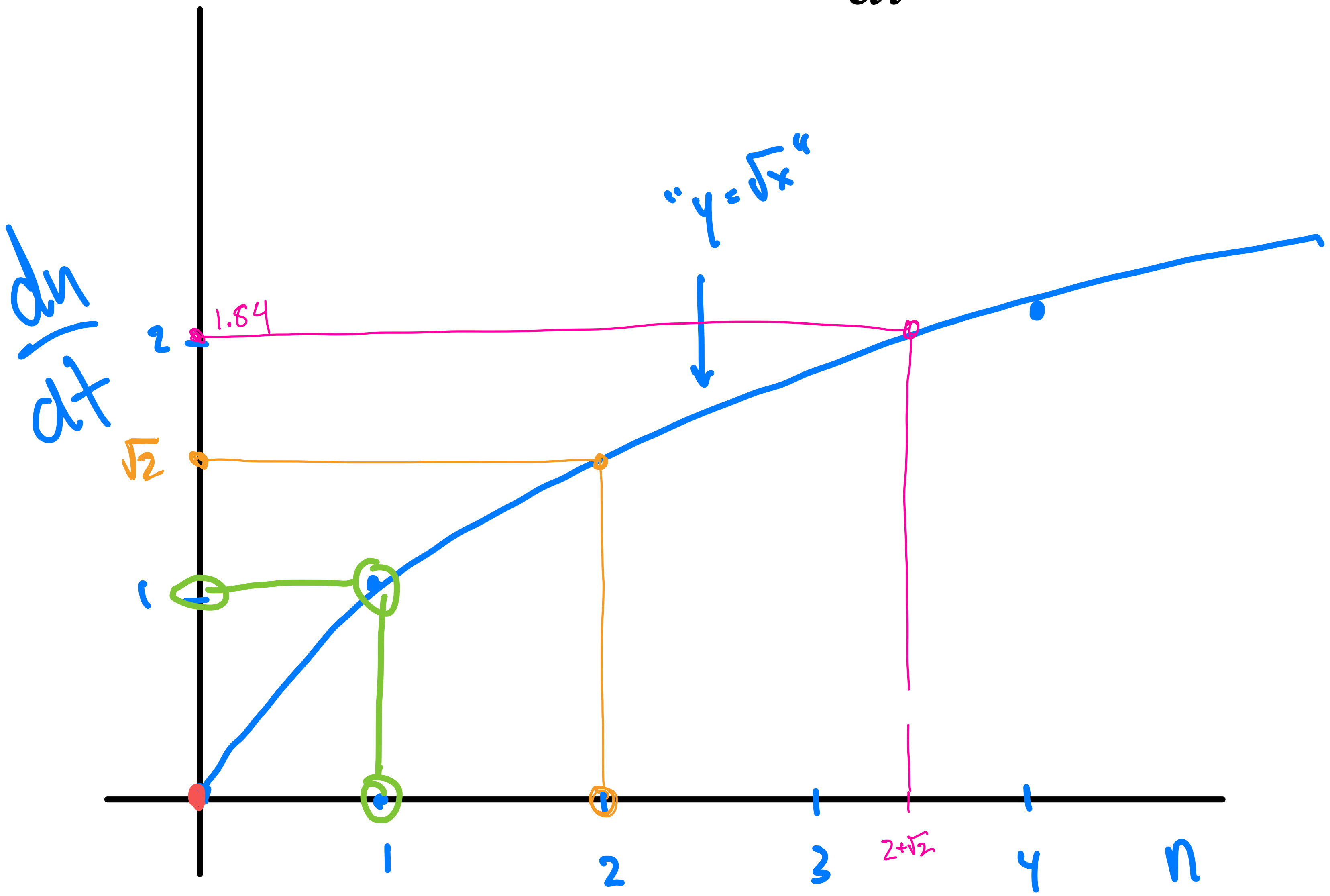
"Forward Euler" Method.

Differential Eq $\longrightarrow$ Recursion Eq.

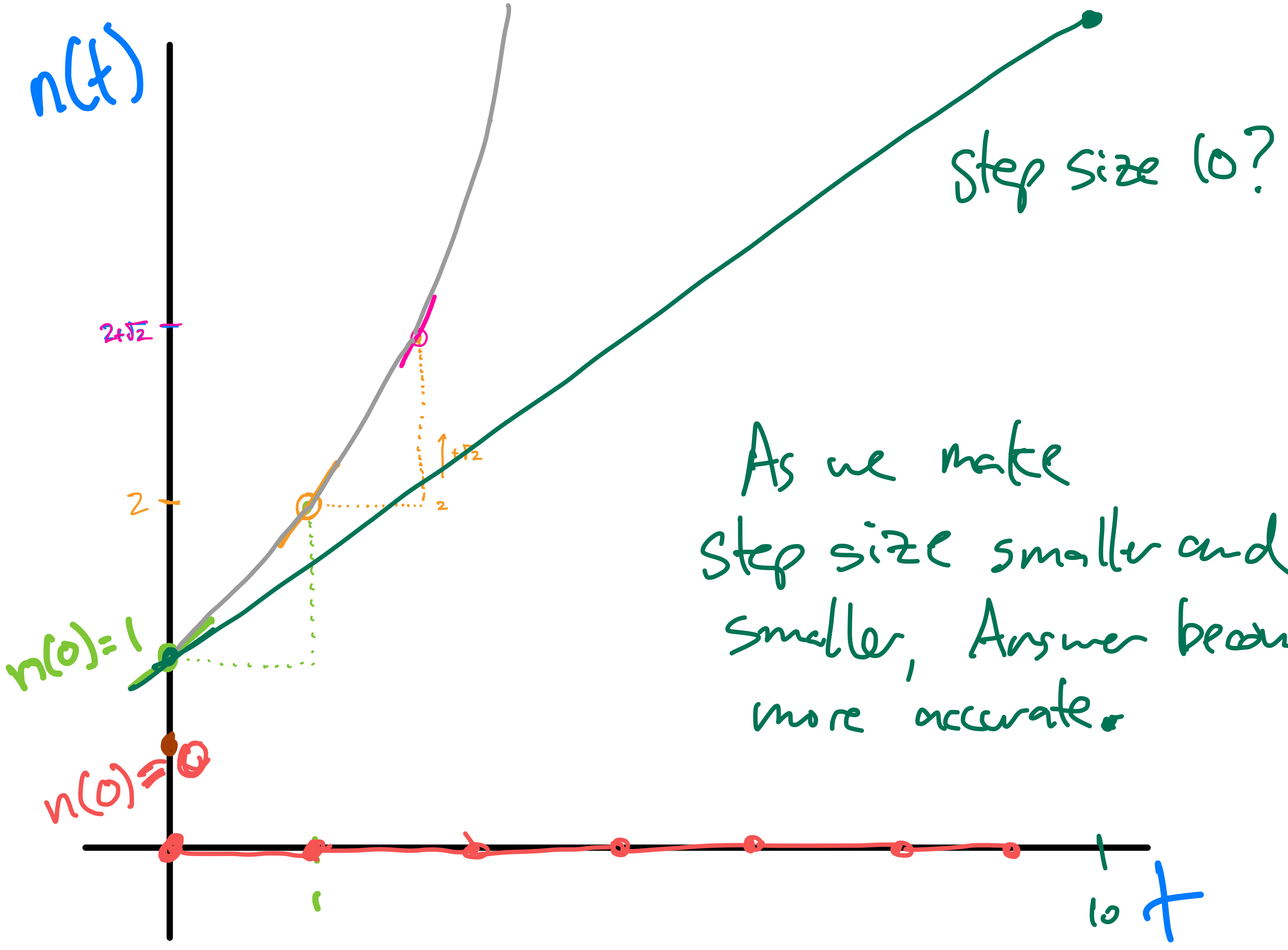
numerical solution "GPS"

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

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



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



As we make step size smaller and smaller, Answer becomes more accurate.

Parameters

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

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

$$n(t+1) = n(t) + r\,n(t)$$

- Branches per month per existing branch — b
- Fraction of mice that die by cat per day — d (death)
- # mice born per day per existing mouse — b (birth)
- Rate of contacts per potential interaction per day. — c
- Probability of transmission per exposure/contact. — a

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.

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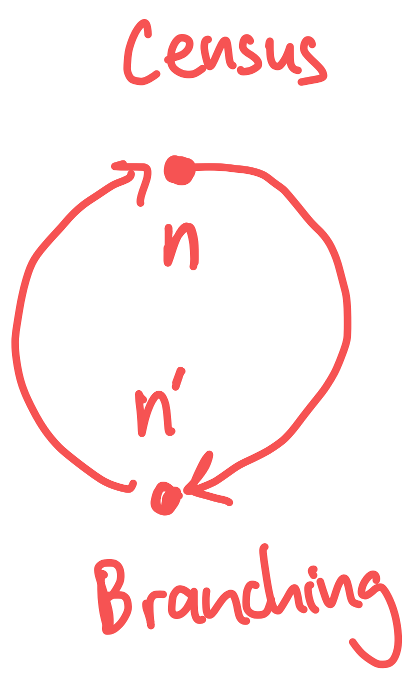
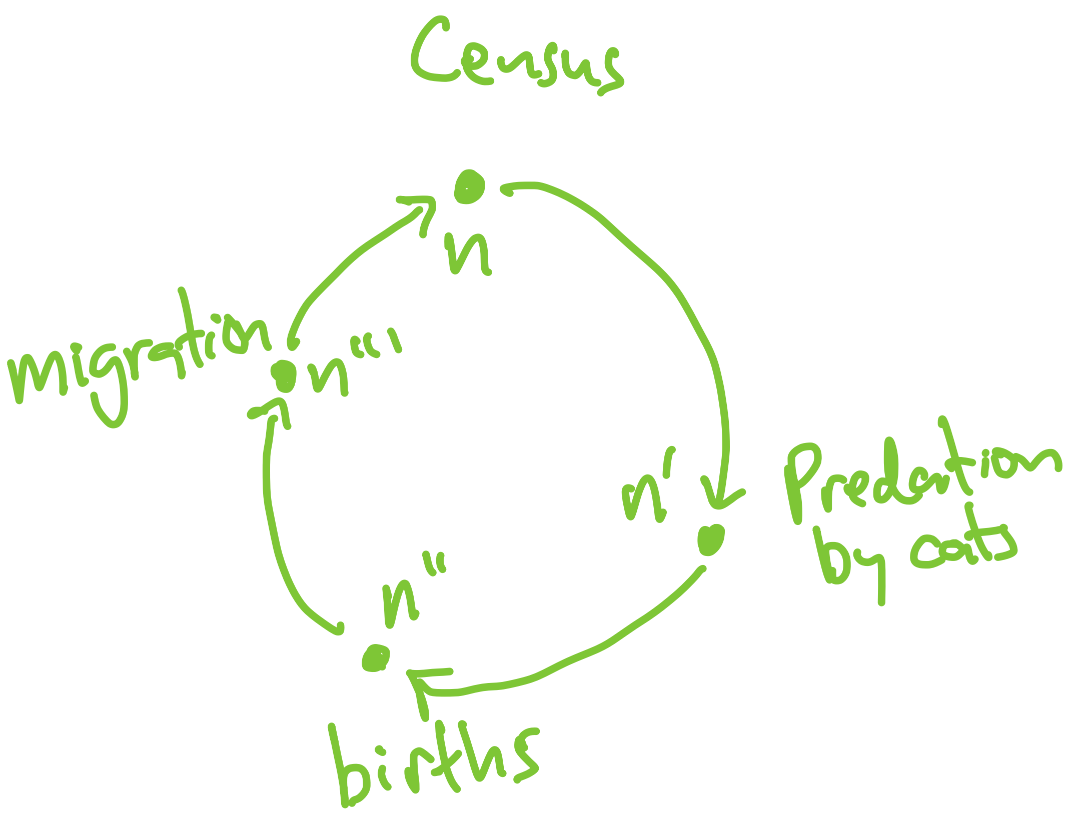
Diagrams: Life Cycle

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

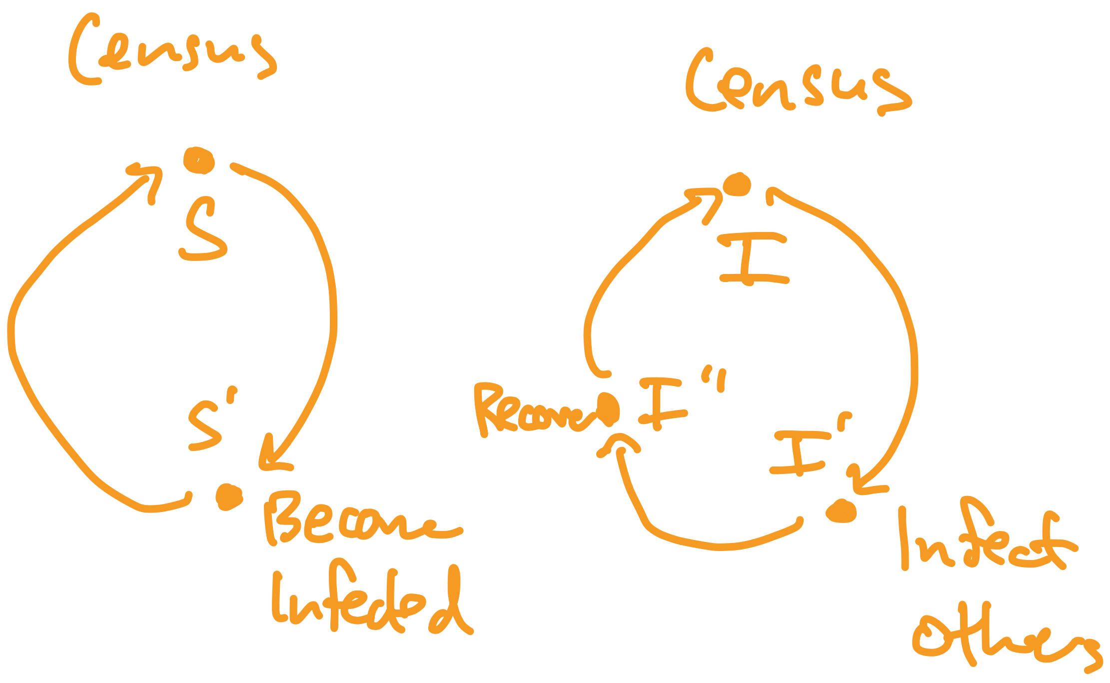
Tree Branches



Mice in Yard



Inf. Dis.

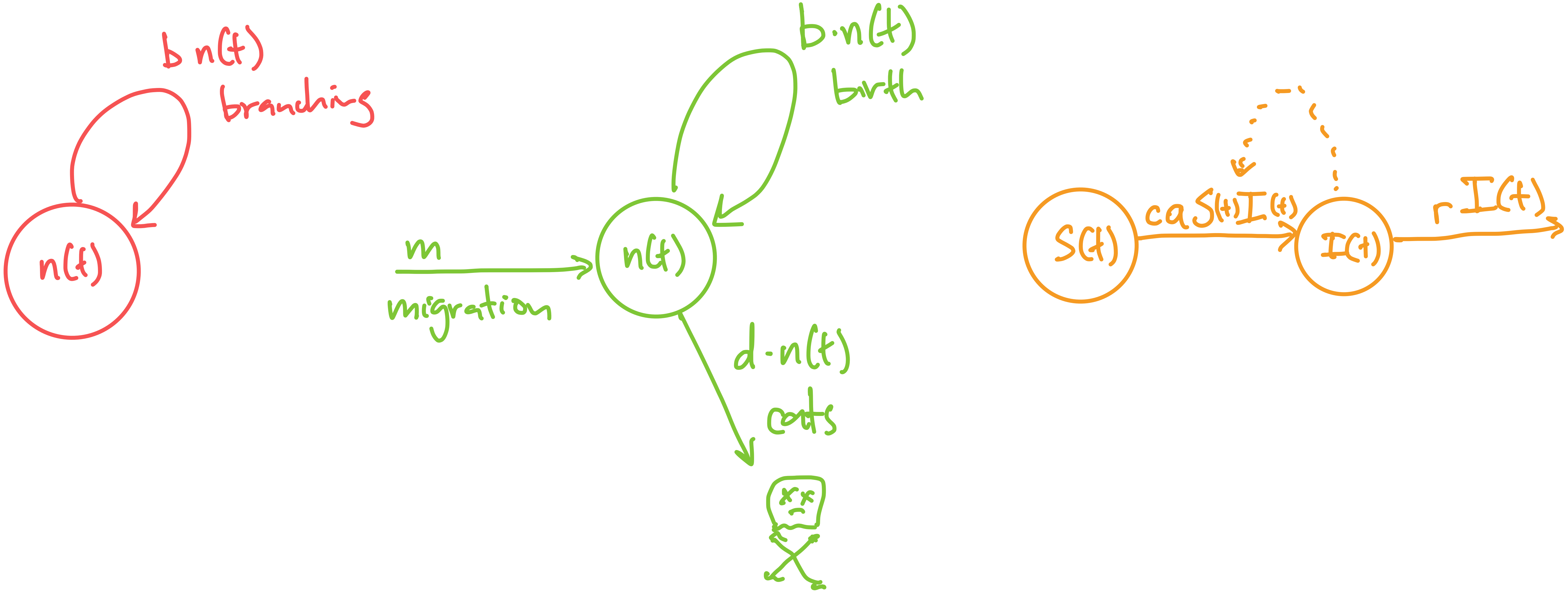


Order matters

tracked multiple variables

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**.

Interaction	# events	Result of Event
$S \times S$	cSS	—
$I \times I$	cII	—
$S \times I$	cSI	$\underline{I}$: $+a$; $\underline{S}$: $-a$

Pros and Cons?

- See Otto & Day, Chapter 2.4

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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 $\Delta n = n(t+1) - n(t) = \ldots$

Example: COVID-19

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

Recipes: differential equations from flow diagrams

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

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

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