Week 8

Mathematics and Computational Methods for Complex Systems, 2023-2024

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Mid module feedback

Module is too easy

Module is too hard

→ Divide notebooks into core + extended

Ask for extra if you like!

Lectures not long/ detailed enough → Happy to take questions at the end

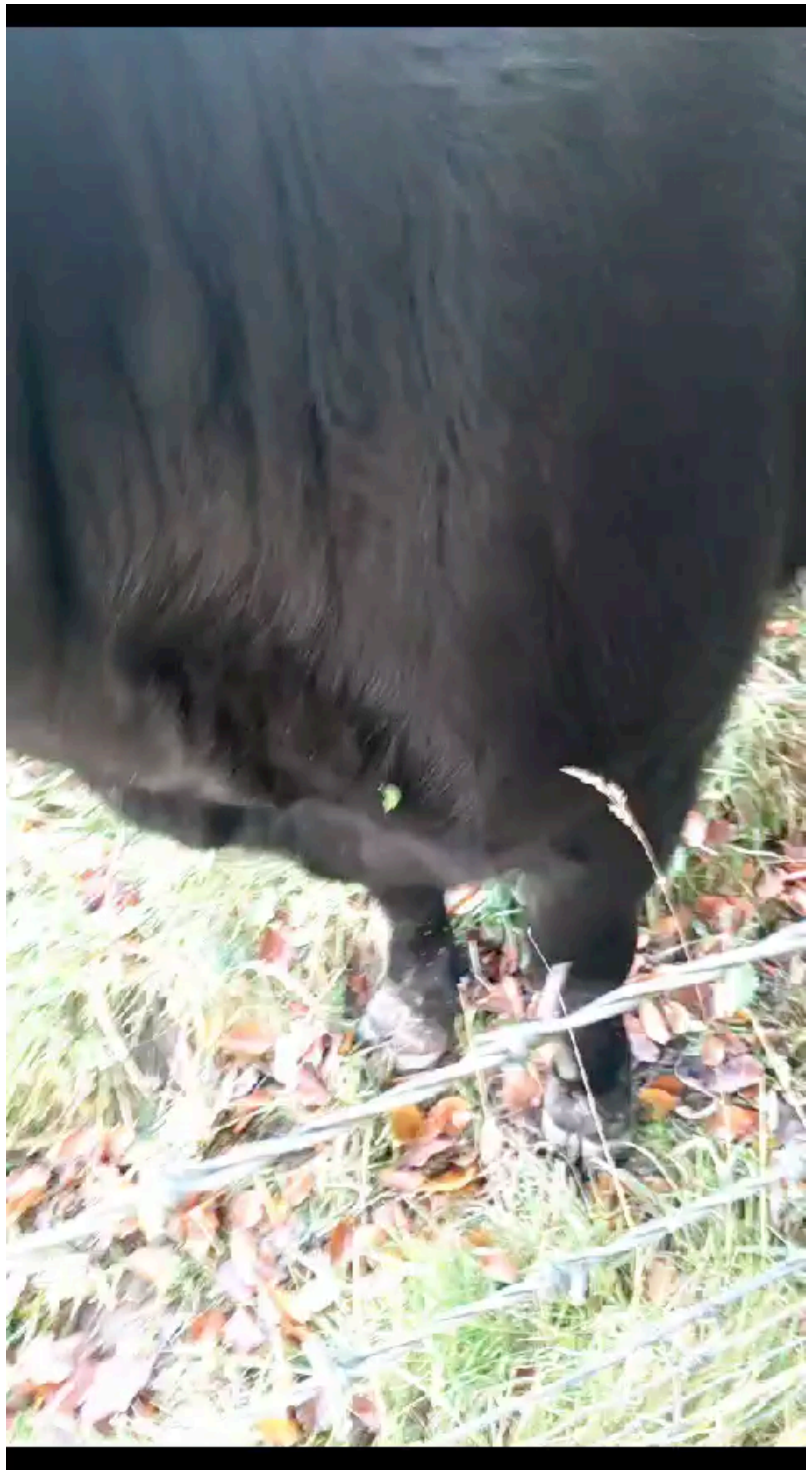
Online resources!

Goals unclear → Recap today

Should be in Python → Exam in either, parallel notebooks

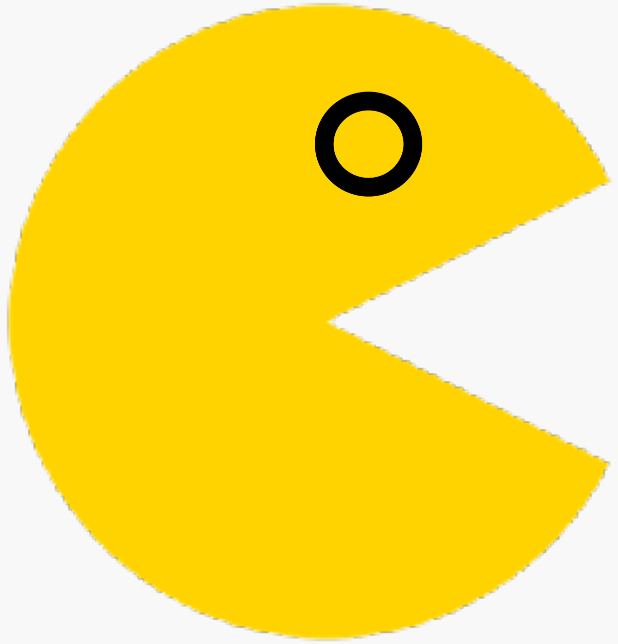
Identical coding patterns!
Teething issues

Reminder on course goals



Reminder on course goals

21st century life



How to learn/communicate/use/think with mathematical concepts

By learning maths!

Learn maths all of it!

Exam

Take home in December

Give back in January

Preparation?

Practice doing maths, not rote-learning

Dynamical systems

Learning dynamical systems
requires experimentation

Play lots with the
code!

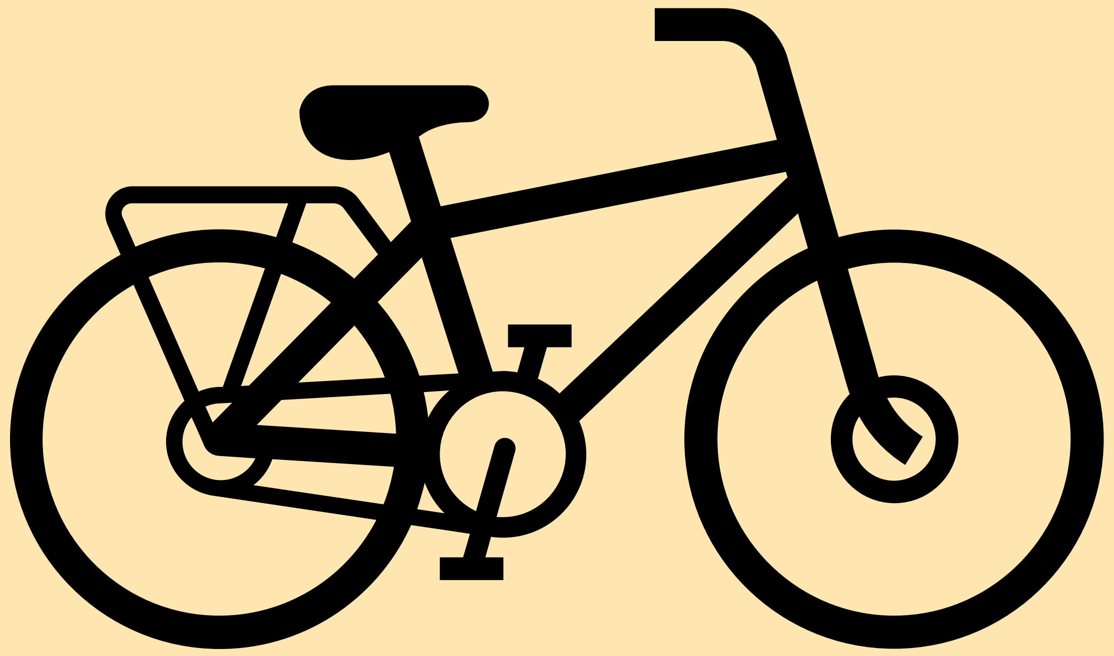
Goal today

Model a pandemic!

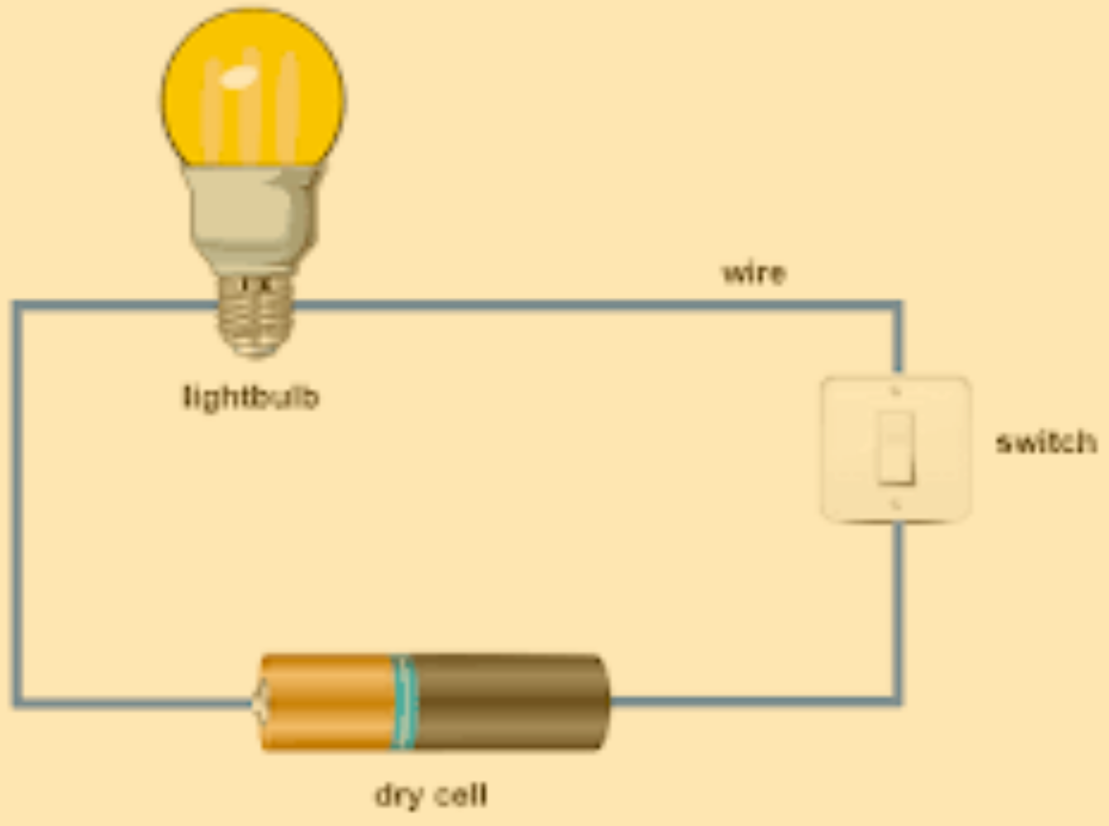
What is a dynamical system

(Intuition)

Something that changes in time
in a constrained way
(so everything)



Laws (constraints)
of mechanics

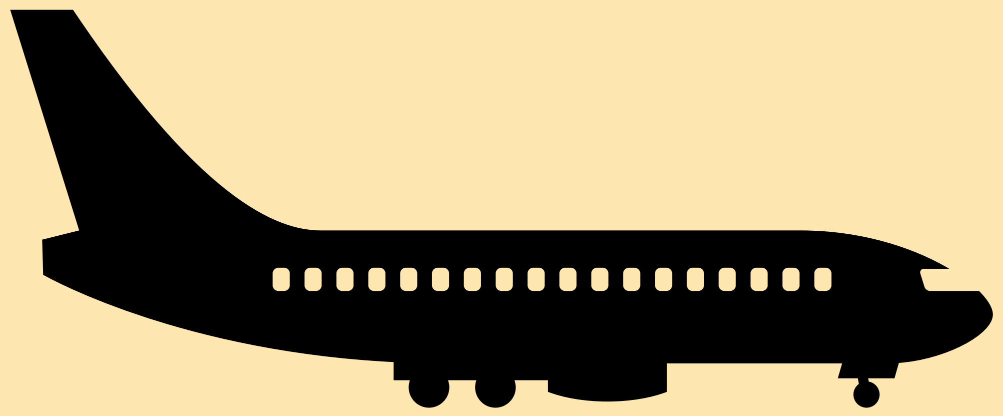


Laws of
electromagnetism

Laws of chemistry,
mechanics, electro…

What do we want to do with dynamical systems?

Analyse

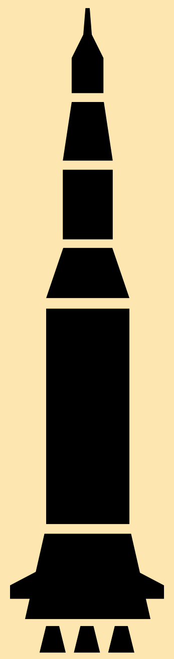


“Won’t crash in high winds”

Predict

“Clouds and light rain tomorrow”

Design



“Make it more fuel-efficient”

We need mathematical models of these systems

How do we model dynamical systems?

Markov process

Hybrid system

Stochastic differential equation

Reaction rate network

Partial differential equation

In this course

(Ordinary) differential equations

(Difference equations)

ODE

Recap

Suppose I am walking with velocity 4m/s

What is $x(t)$, my position as a function of time?

Recap

Velocity is rate of change of position with respect to time:

$$\frac{\mathrm{d}x}{\mathrm{d}t}(t)$$

Maths problem: need to solve

$$\frac{\mathrm{d}x}{\mathrm{d}t}(t) = 4$$

This is a differential equation

"Differential"
quantity

$$\boxed{\frac{\mathrm{d}x}{\mathrm{d}t}}(t) = 4$$

Equations that include differential quantities
(i.e. derivatives)

What are we trying to do

Information on differential quantity over all time

$$\frac{\mathrm{d}x}{\mathrm{d}t}(t) = 4$$

“Solution”

Information on quantity itself over all time

$$x(t) = ?$$

Solution terminology

General solution

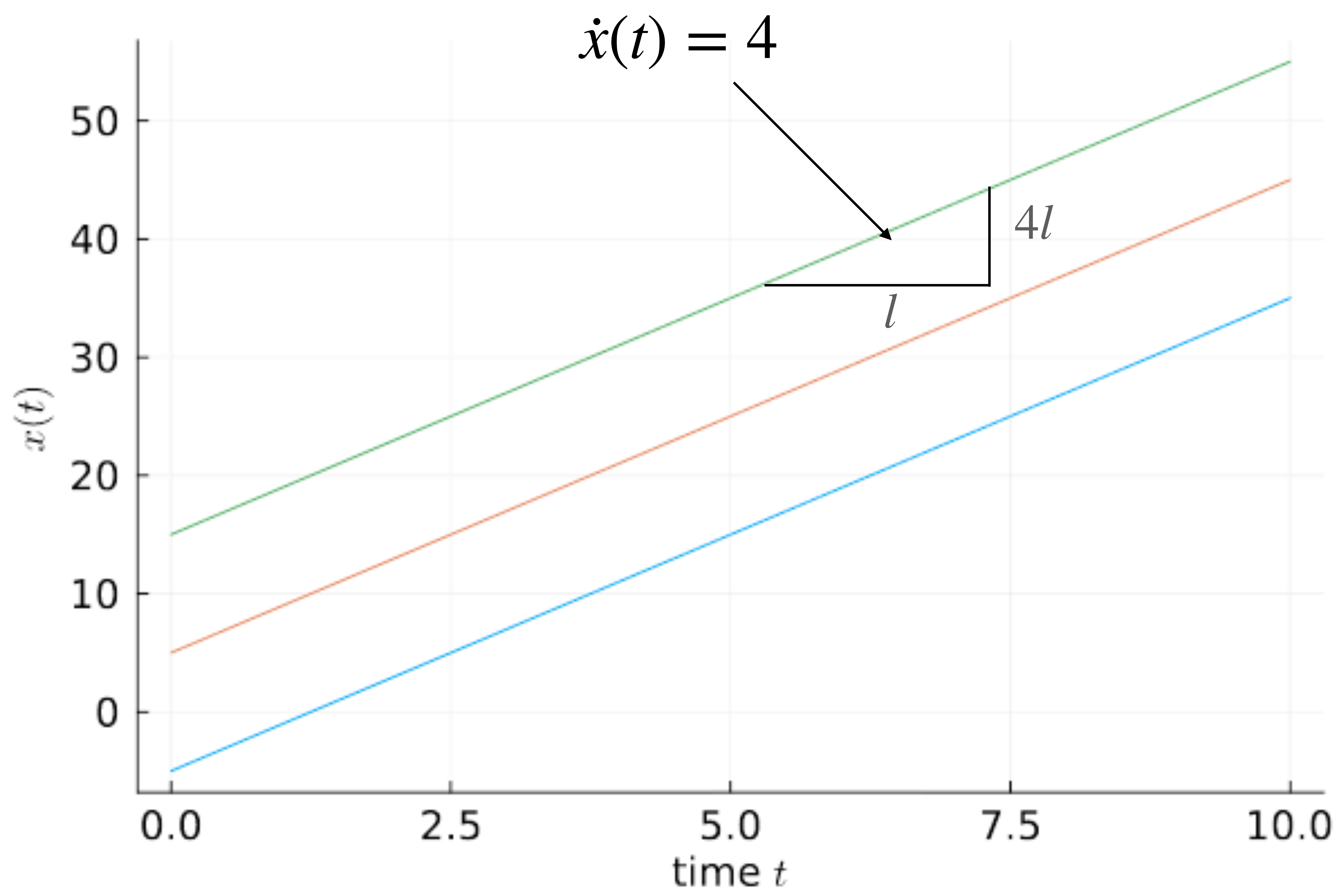
$x(t) = 4t + C$

Constant of integration

Particular solution

$x(t) = 4t + 15$

“Integrating the differential equation”



Initial conditions allow us to pick a particular solution

General solution

$x(t) = 4t + C$

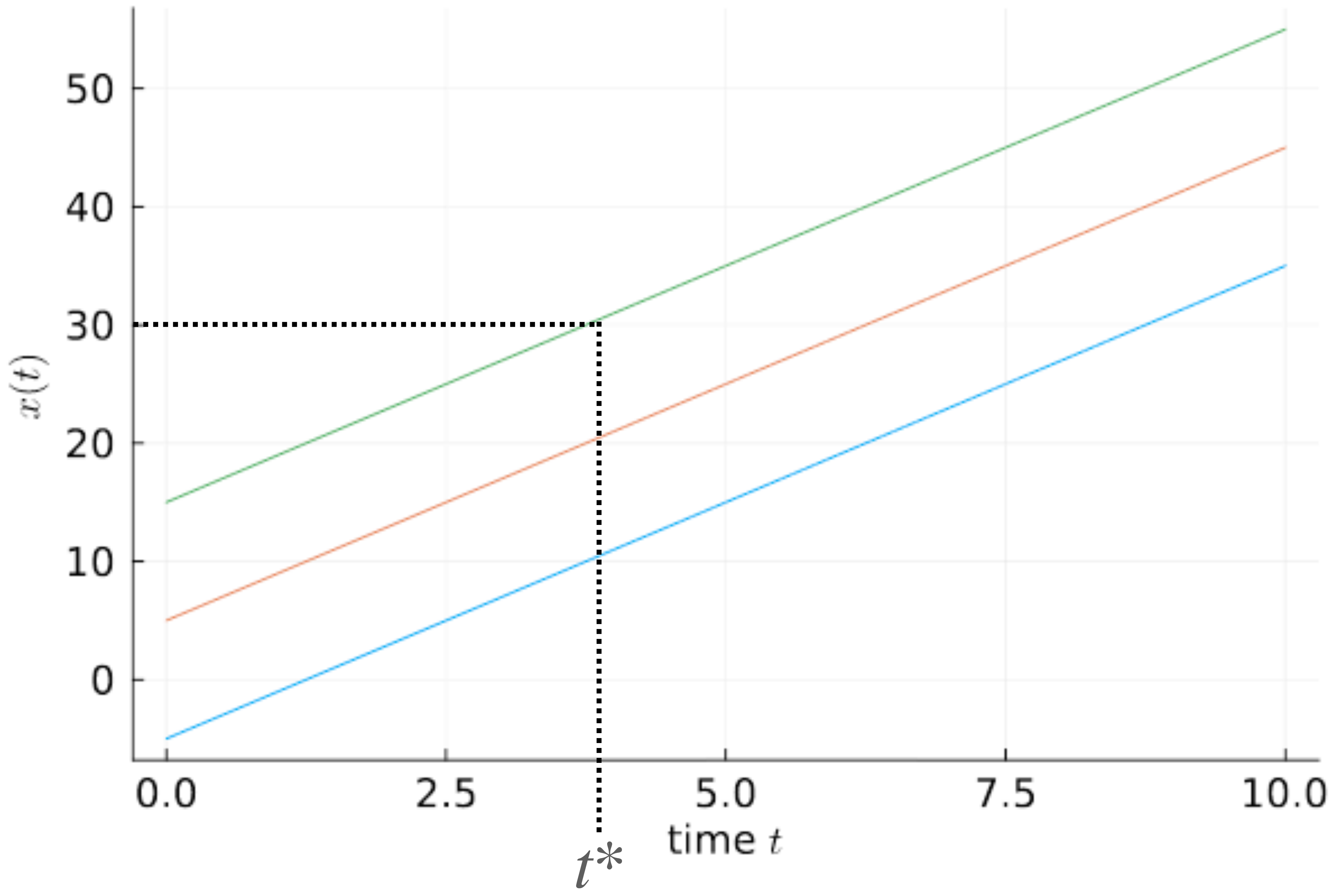
Particular solution

$x(t) = 4t + 15$

Initial conditions

$$x(t^*) = 40$$

(Usually $t^* = 0$)



What it means to solve a Differential Equation

How something changes

Suppose I am walking with velocity 4m/s

+

What something is at some time

Initial position is 2m

→

What something is over all time

What is my position as a function of t?

What it means to solve a Differential Equation

How something changes

Suppose I am walking with velocity 4m/s

+

What something is at some time

Initial position is 2m

→

What something is over all time

What is my position as a function of t?

Differential equation

$$\dot{x}(t) = 4$$

+

"Initial Condition"

$$x(0) = 15$$

→

Solution: function of time

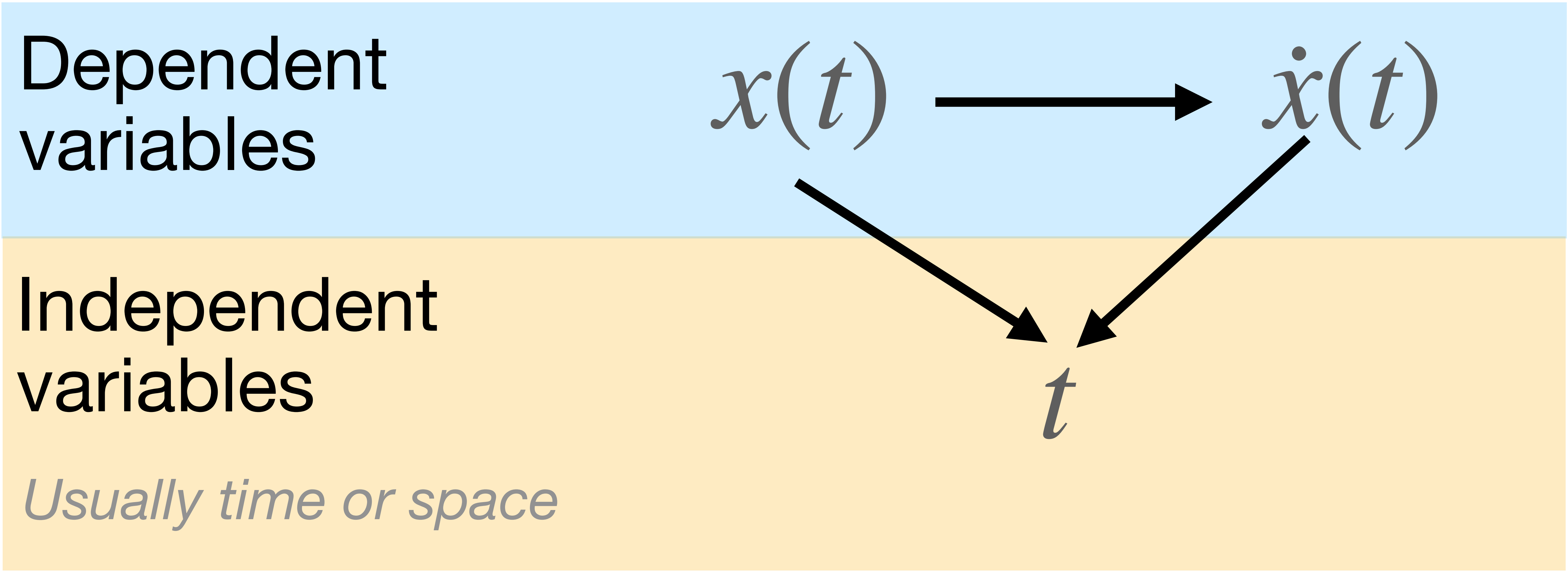
$$x(t) = 4t + 15$$

Also called an initial value problem

Classification of variables

$$\dot{x}(t) = 4$$

Variable dependencies



- Denominators in the derivatives

Sketch this differential equation

$$\dot{x}(t) = x(t)$$

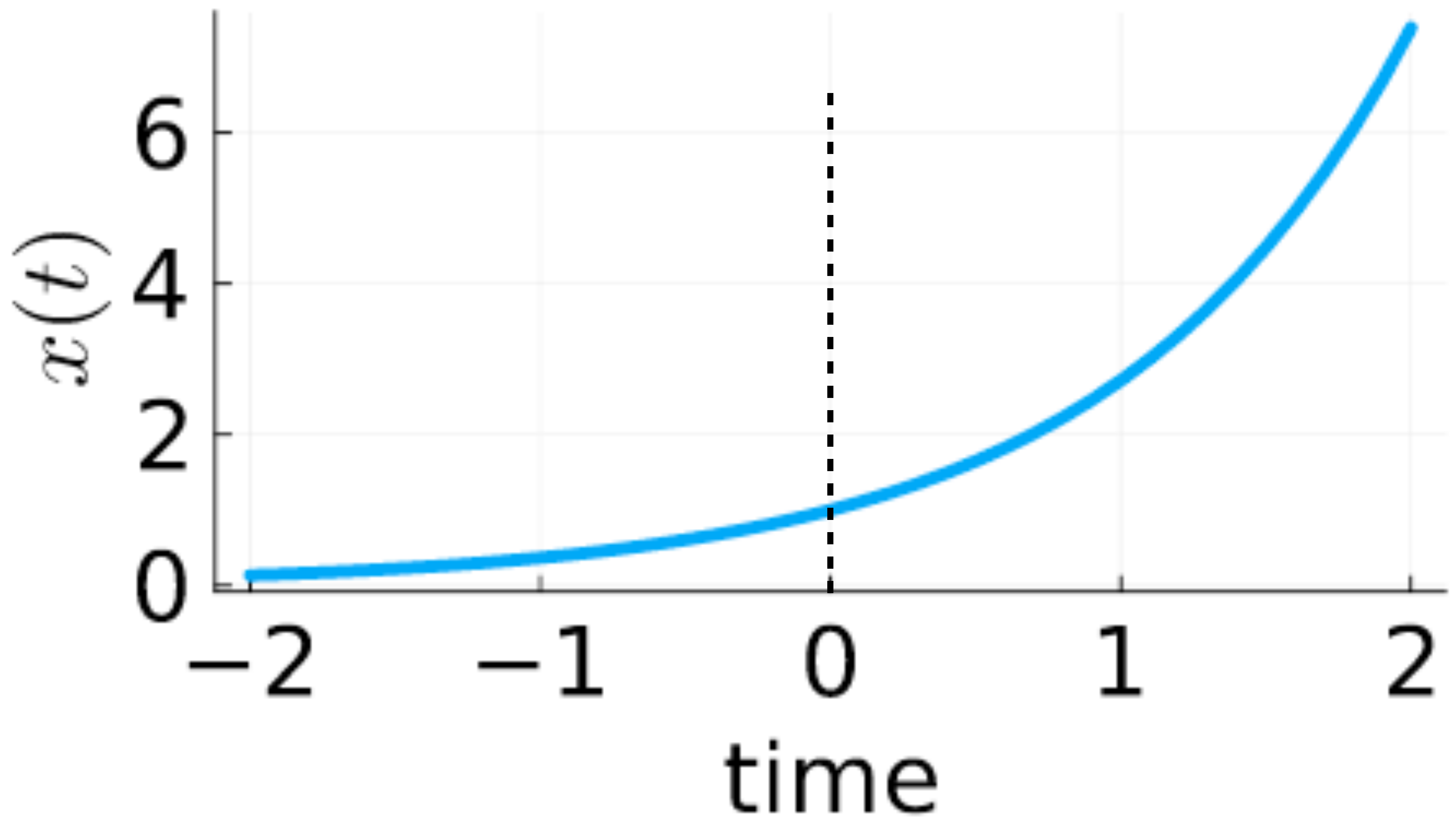
$$x(0) = 1$$

Option 0: educated guesswork

Important skill!

$$\dot{x}(t) = x(t)$$

$$x(0) = 1$$



Derivative starts positive, so function is increasing at zero

If function increases then derivative increases

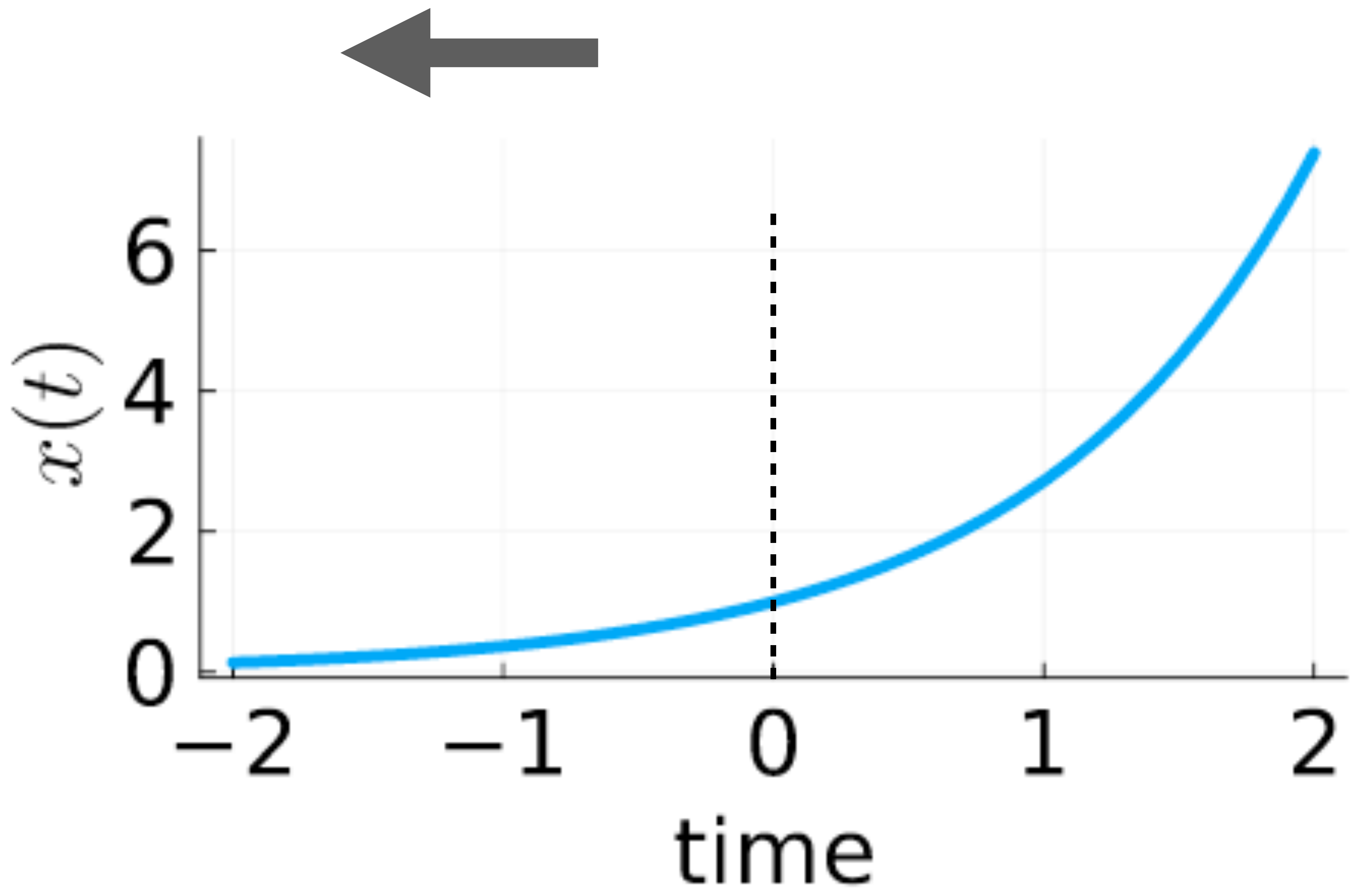
Positive feedback: function accelerates

Option 0: educated guesswork

Important skill!

$$\dot{x}(t) = x(t) \qquad x(0) = 1$$

$$\frac{\mathrm{d}x}{\mathrm{d}(-t)} = -\frac{\mathrm{d}x}{\mathrm{d}(t)}$$ (chain rule)



Derivative starts positive, so function is increasing at zero

If function increases then derivative increases

Positive feedback: function accelerates

Sketch the same differential equation

…with different initial conditions

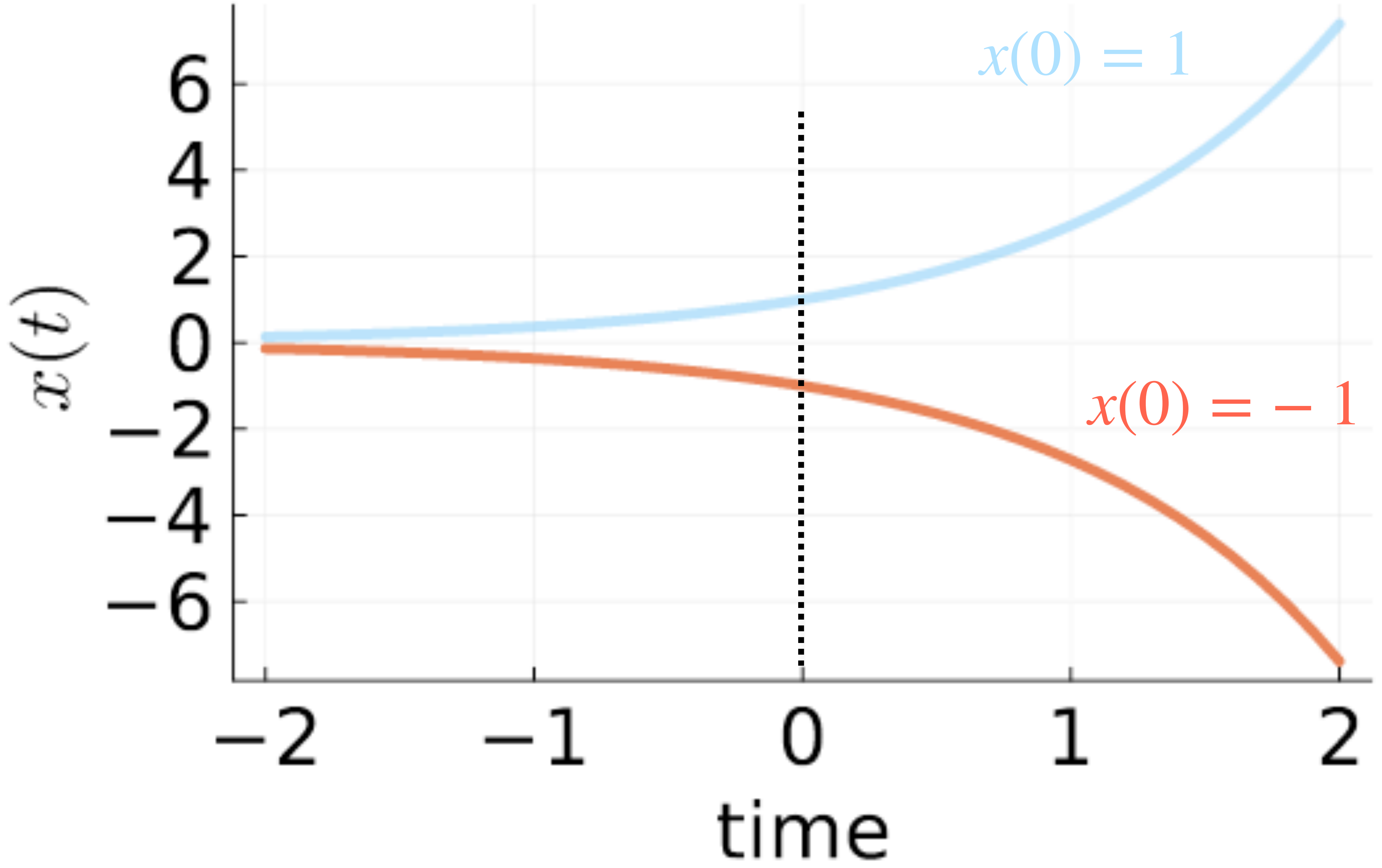
$$\dot{x}(t) = x(t)$$

$$x(0) = -1$$

Small differences in initial conditions can have a big effect

$$\dot{x}(t) = x(t)$$

$$x(0) = -1$$



Derivative starts negative, so function is decreasing at zero

If function decreases then derivative decreases

Positive feedback: function accelerates

Option 1: analytical solution

Usually impossible

$$\frac{\mathrm{d}x}{\mathrm{d}t} = x(t)$$

$$x(0) = 1$$

$$\Rightarrow \frac{1}{x(t)}\mathrm{d}x = 1\mathrm{d}t$$

$$\Rightarrow \ln(x(t)) = t + C$$

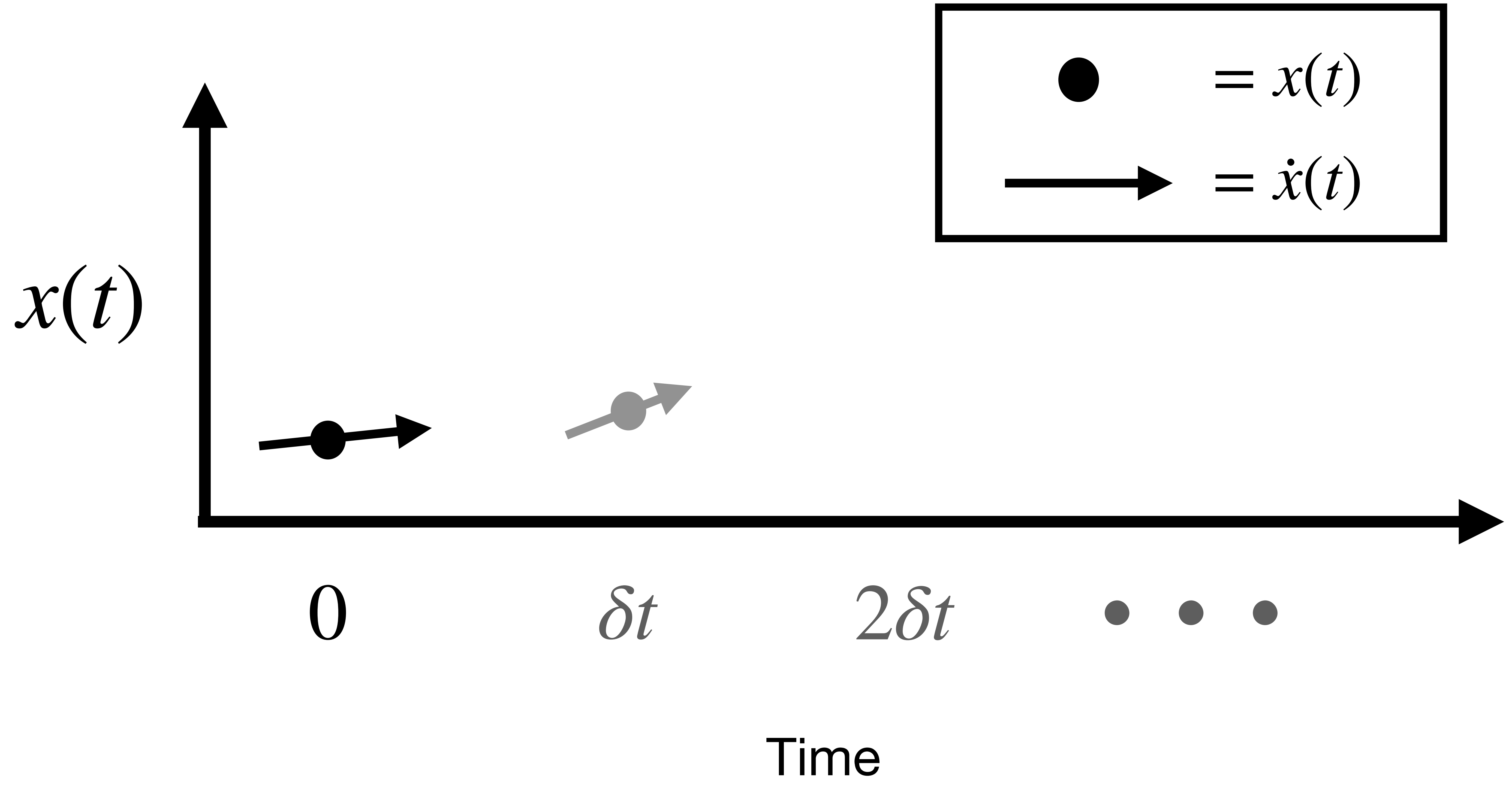
Constant of integration

$$\Rightarrow x(t) = x(0)\exp(t)$$

$$(x(0) = \exp(C))$$

Option 2: numerical solution

Predict $x(t + \delta t)$ ***from*** $x(t)$ ***and*** $\dot{x}(t)$



Option 2: numerical solution

Predict $x(t+\delta t)$ *from* $x(t)$ *and* $\dot{x}(t)$

(Finite-difference approximation of derivative)

$$1. \quad \dot{x}(t) \approx \frac{x(t+\delta t) - x(t)}{\delta t}$$

(Rearrange)

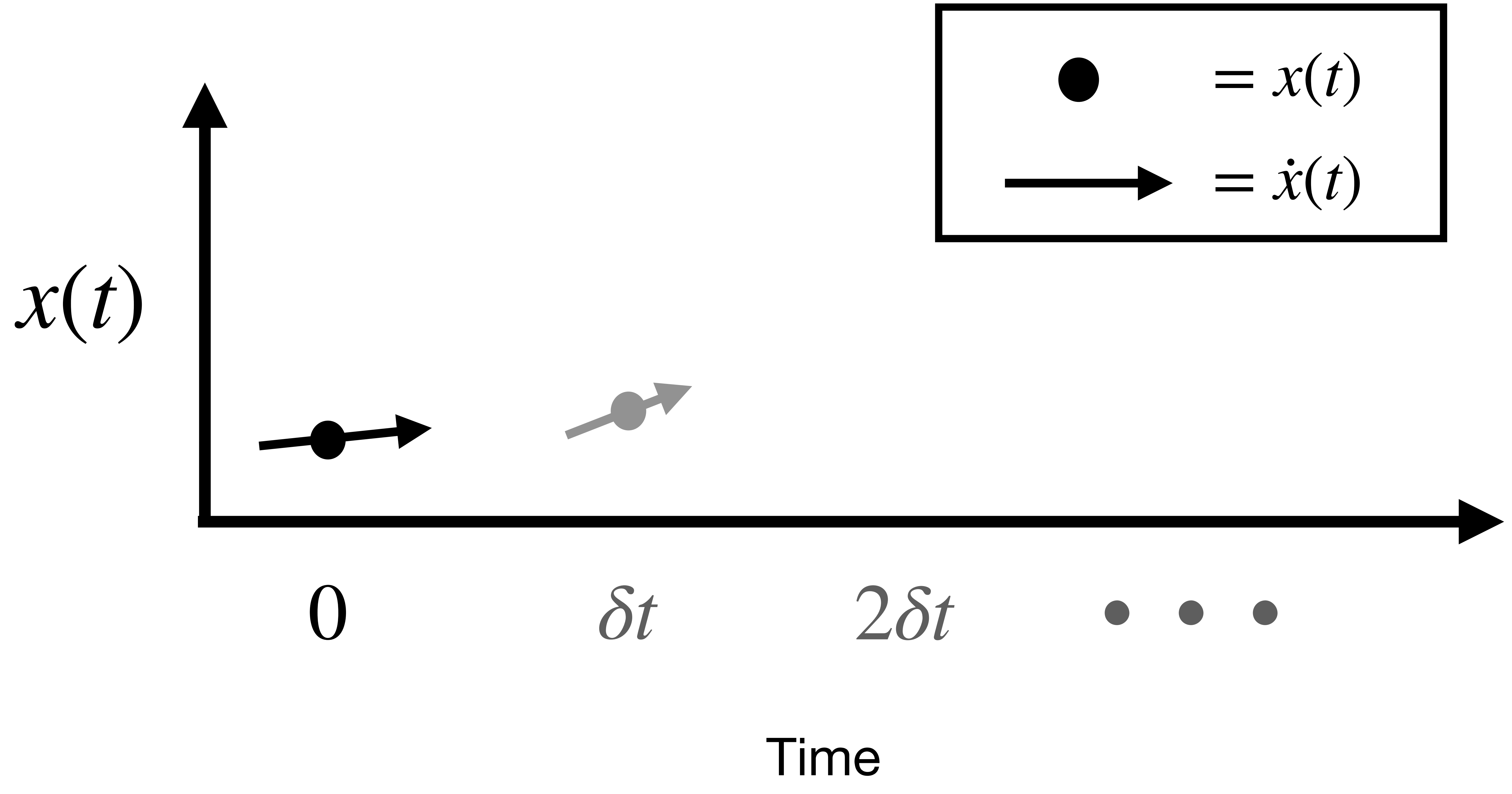
$$2. \quad \underbrace{x(t+\delta t)}_{\text{Predict}} \approx \underbrace{x(t)}_{\text{Know}} + (\delta t)\underbrace{\dot{x}(t)}_{\text{Know}}$$

Option 2: numerical solution

Predict $x(t+\delta t)$ ***from*** $x(t)$ ***and*** $\dot{x}(t)$

$$\underbrace{x(0+\delta t)}_{\text{Predict}} \approx \underbrace{x(0)}_{\text{Know}} + (\delta t)\underbrace{\dot{x}(0)}_{\text{Know}}$$

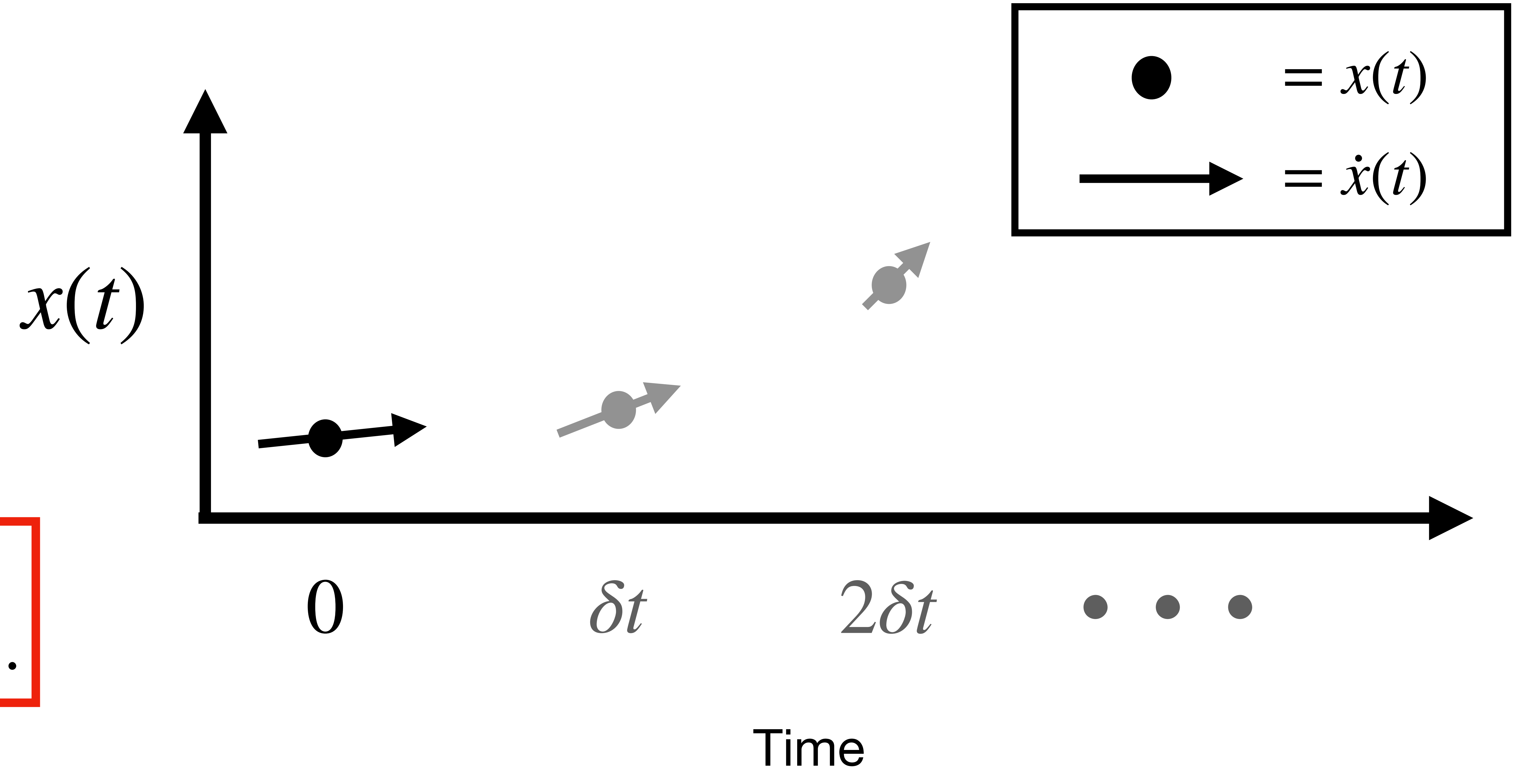
$$\dot{x}(\delta t) = x(\delta t)$$



Option 2: numerical solution

Predict $x(t+\delta t)$ ***from*** $x(t)$ ***and*** $\dot{x}(t)$

$$x(2\delta t) \approx x(\delta t) + [\delta t]\dot{x}(\delta t)$$
$$\dot{x}(2\delta t) = x(2\delta t)$$



Iterate for
$x(t+2\delta t), x(t+3\delta t), \ldots$

General form of first order Ordinary Differential Equations (ODE)

$$\dot{x}(t) = f(x(t), t)$$ Arbitrary function f

$$\dot{x}(0) = x_0$$

Examples

Is first order

$$\dot{x}(t) = [x(t)]^2 + 2tx(t)$$

Isn't first order

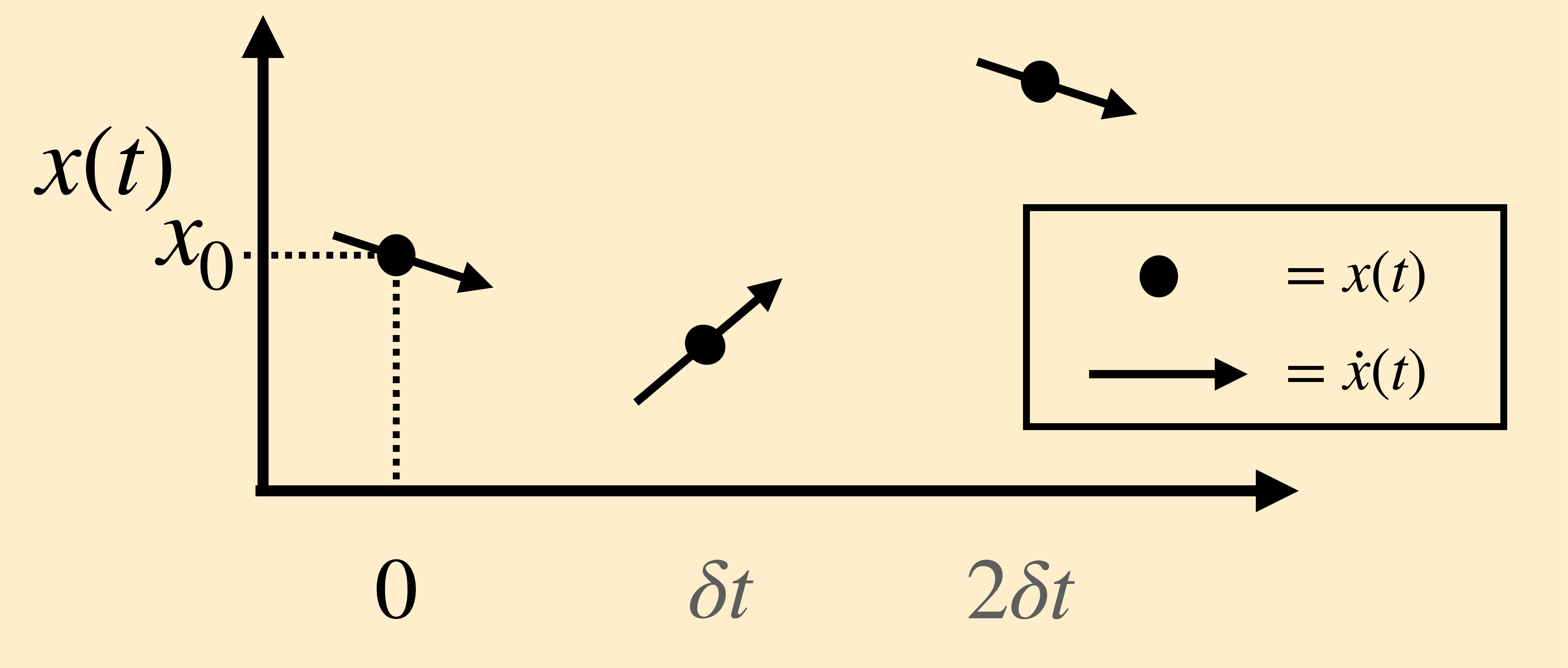
$$\ddot{x}(t) = -x(t)$$

Second order (double derivative)

Forward Euler algorithm for numerically solving first-order ODEs

$$\dot{x}(t) = f(x(t), t)$$

$$\dot{x}(0) = x_0$$



Forward Euler algorithm for numerically solving first-order ODEs

$$\dot{x}(t) = f(x(t), t)$$

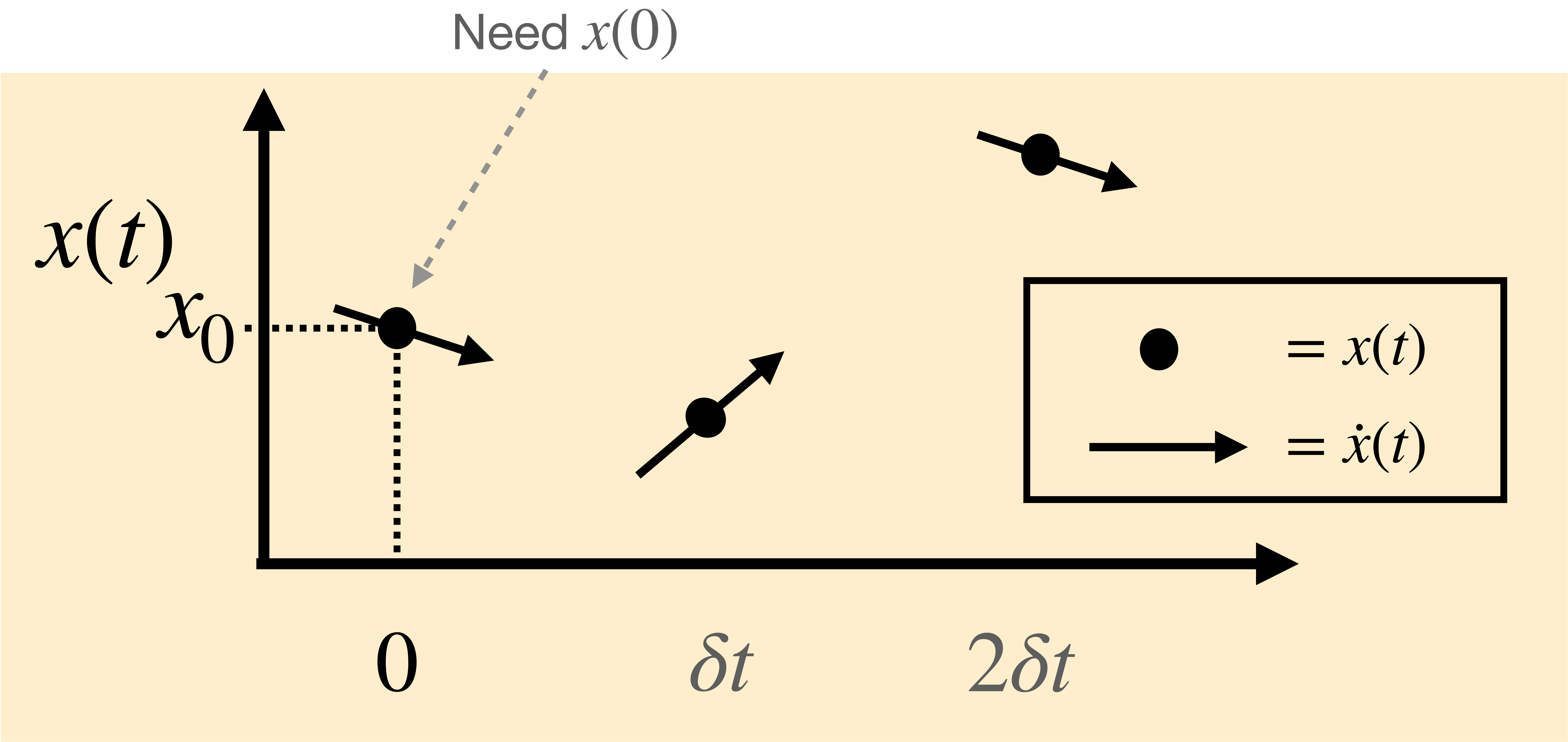
$$\dot{x}(0) = x_0$$

(Julia code in notebook)

```
for t in δt*np.arange(1,n):

    x(t + δt) = x(t) + δt*f(x(t))
```

$= \dot{x}(t)$



Terminology

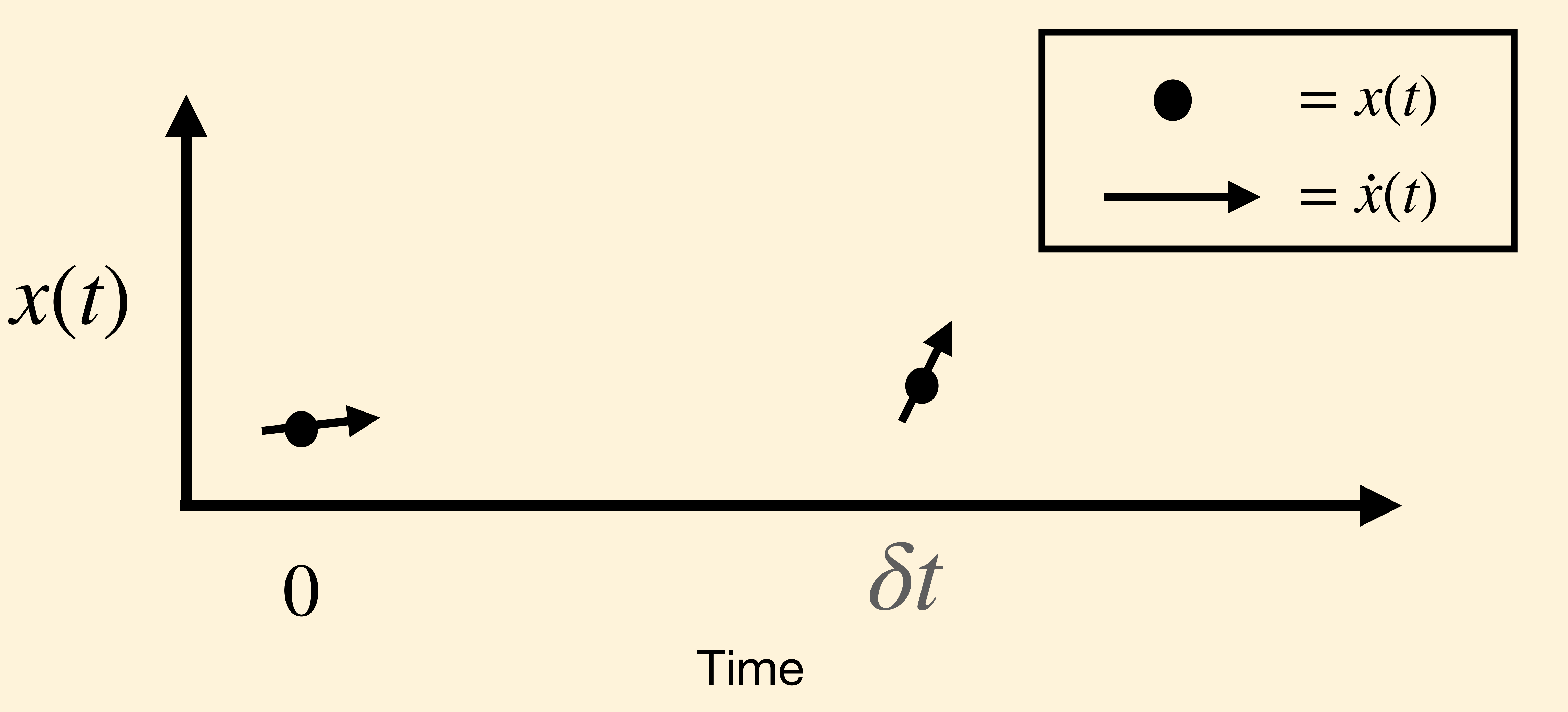
Forward Euler is a “numerical ODE solver”

The simplest but not the best!…

Evaluating numerical solvers

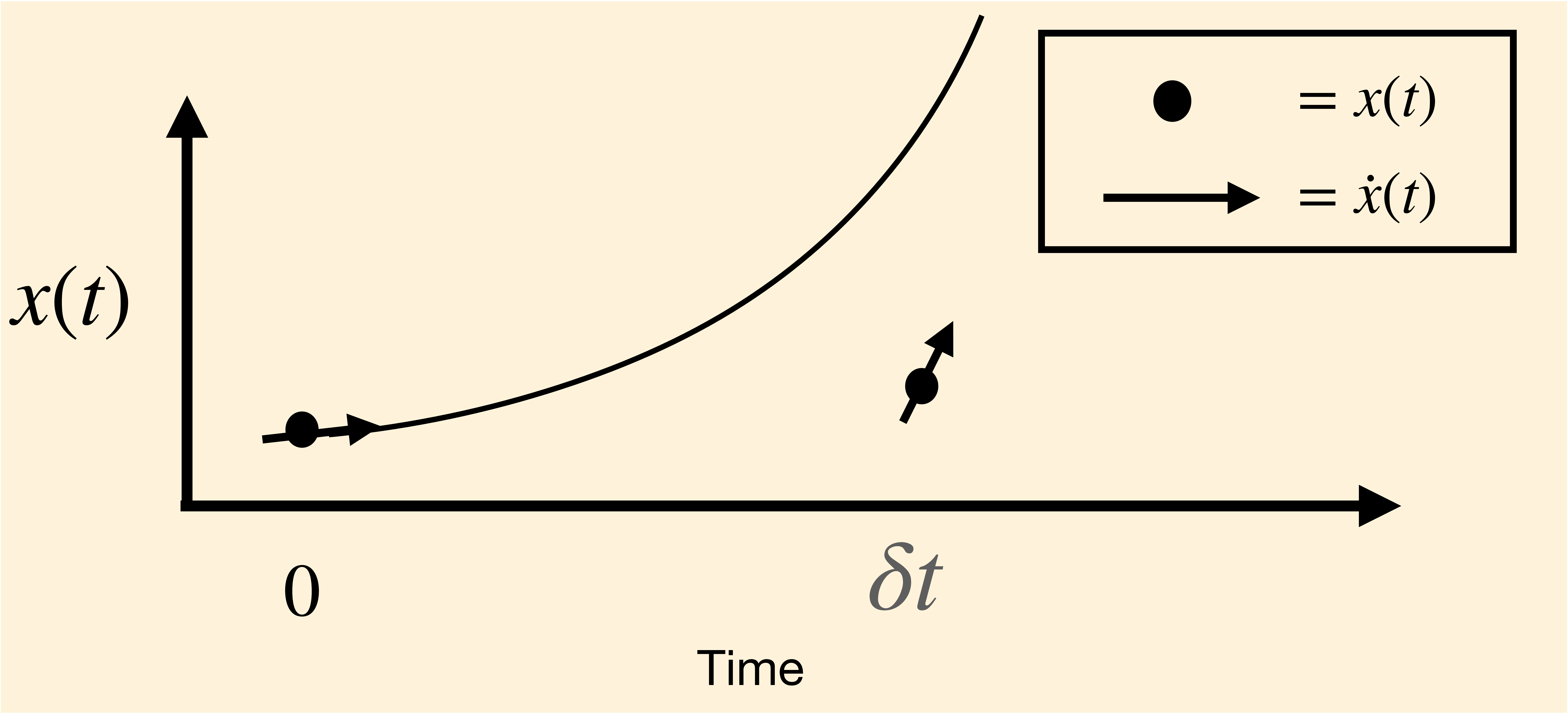
Sources of approximation error?

Is $x(\delta t)$ an over or under-estimate in this example?



Evaluating numerical solvers

Numerical approximation was an over-estimate



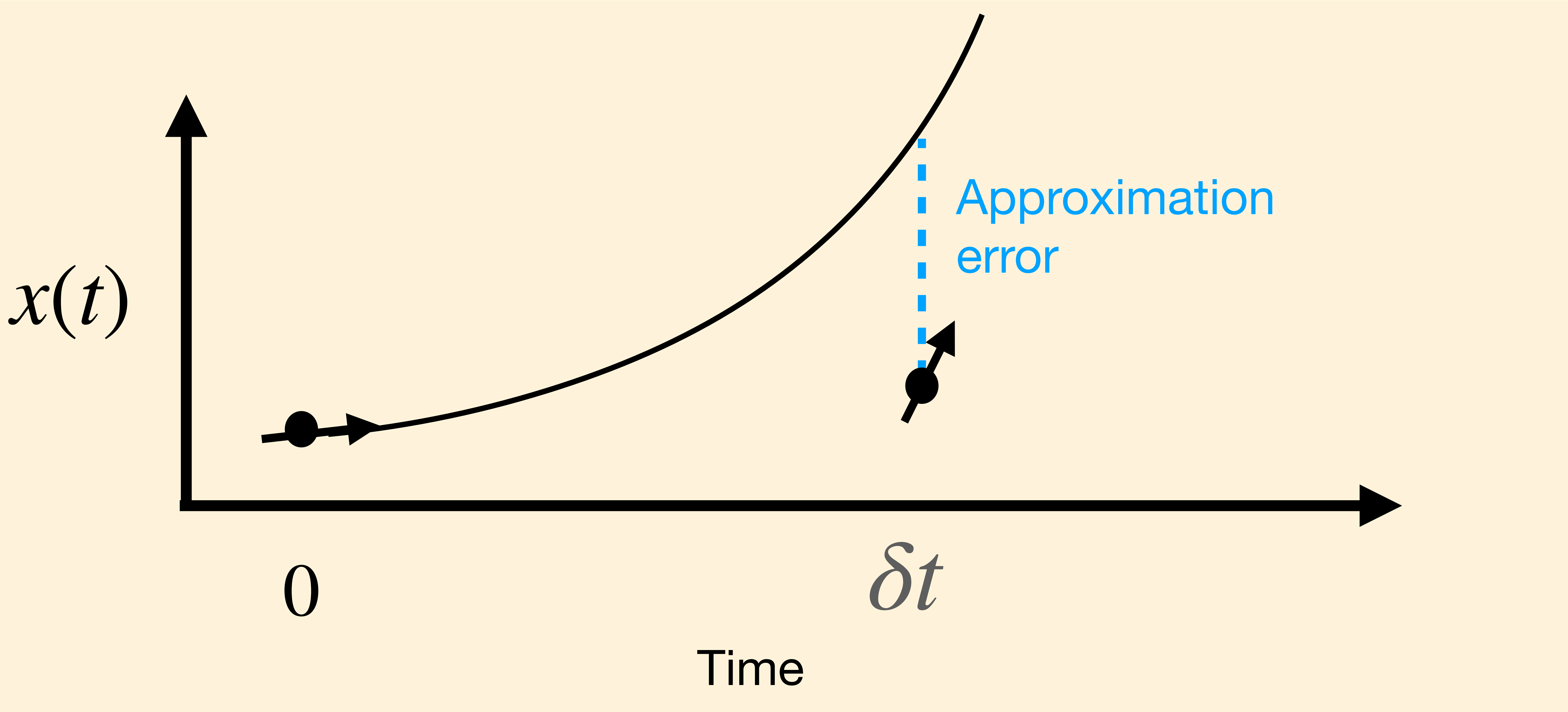
Derivative increases over interval

Function increases faster than $\dot{x}(0)$ suggests

Diagnostic: $\dot{x}(\delta t) > \dot{x}(0)$

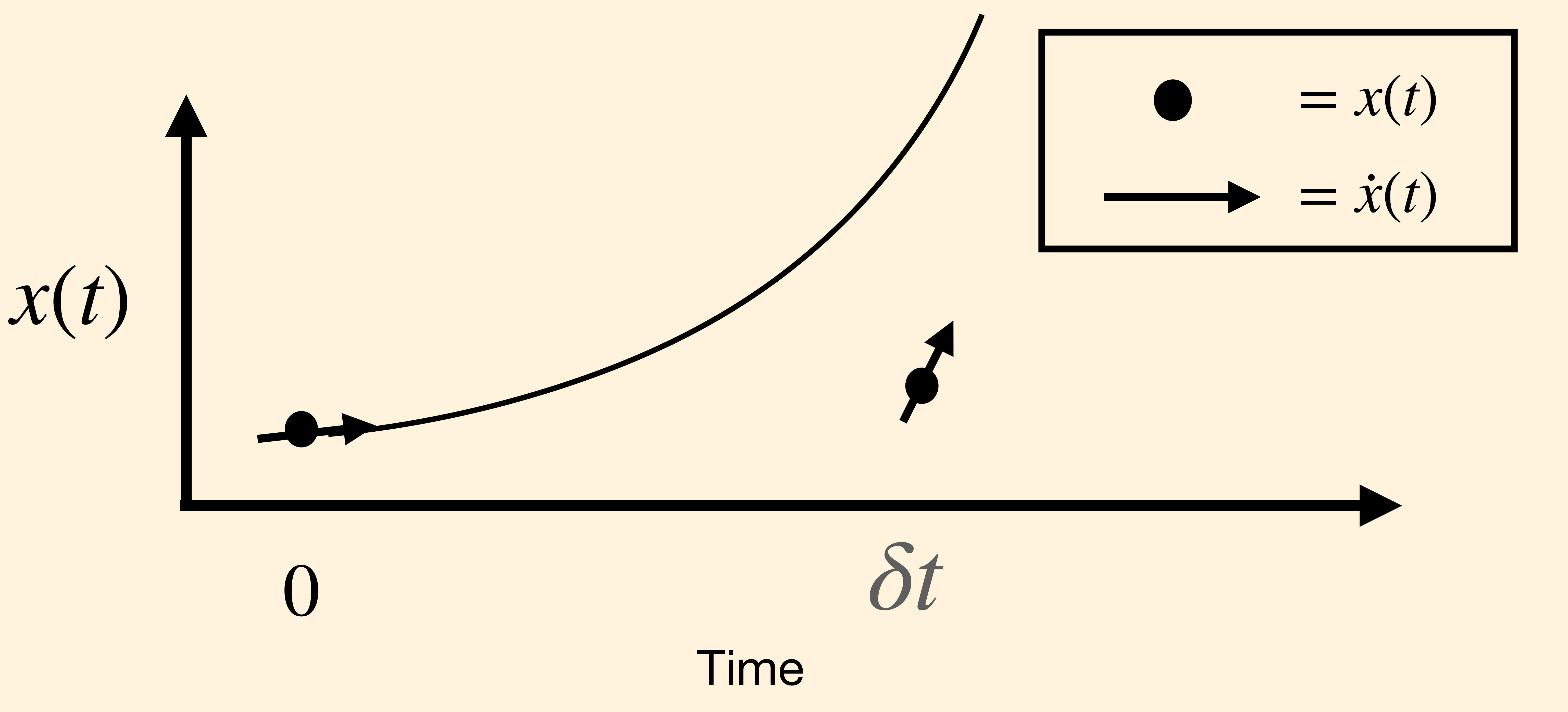
Evaluating numerical solvers

What could decrease approximation error?



Evaluating numerical solvers

What could decrease approximation error?



Clever

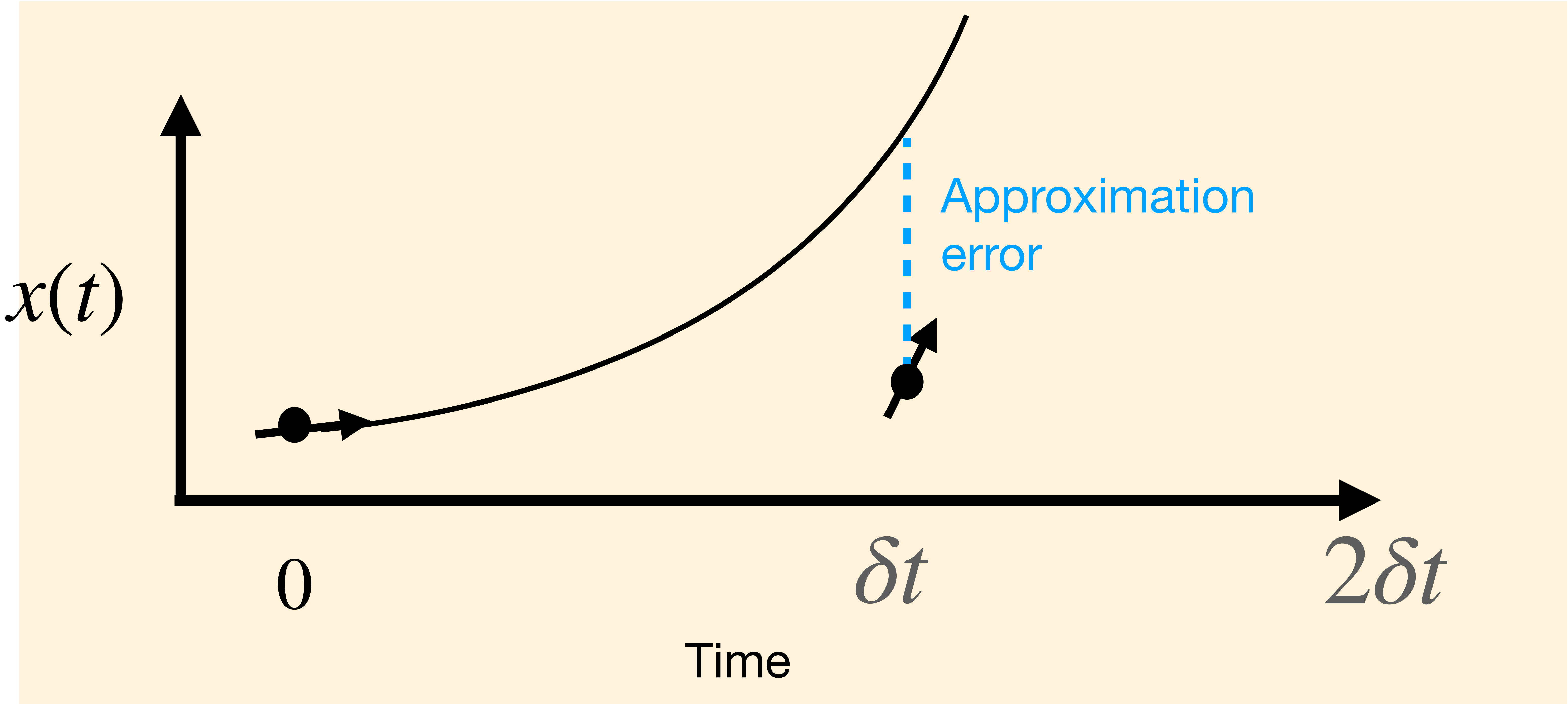
Change in a direction that interpolates $\dot{x}(0)$ and $\dot{x}(\delta t)$

Brute force

Decrease δt

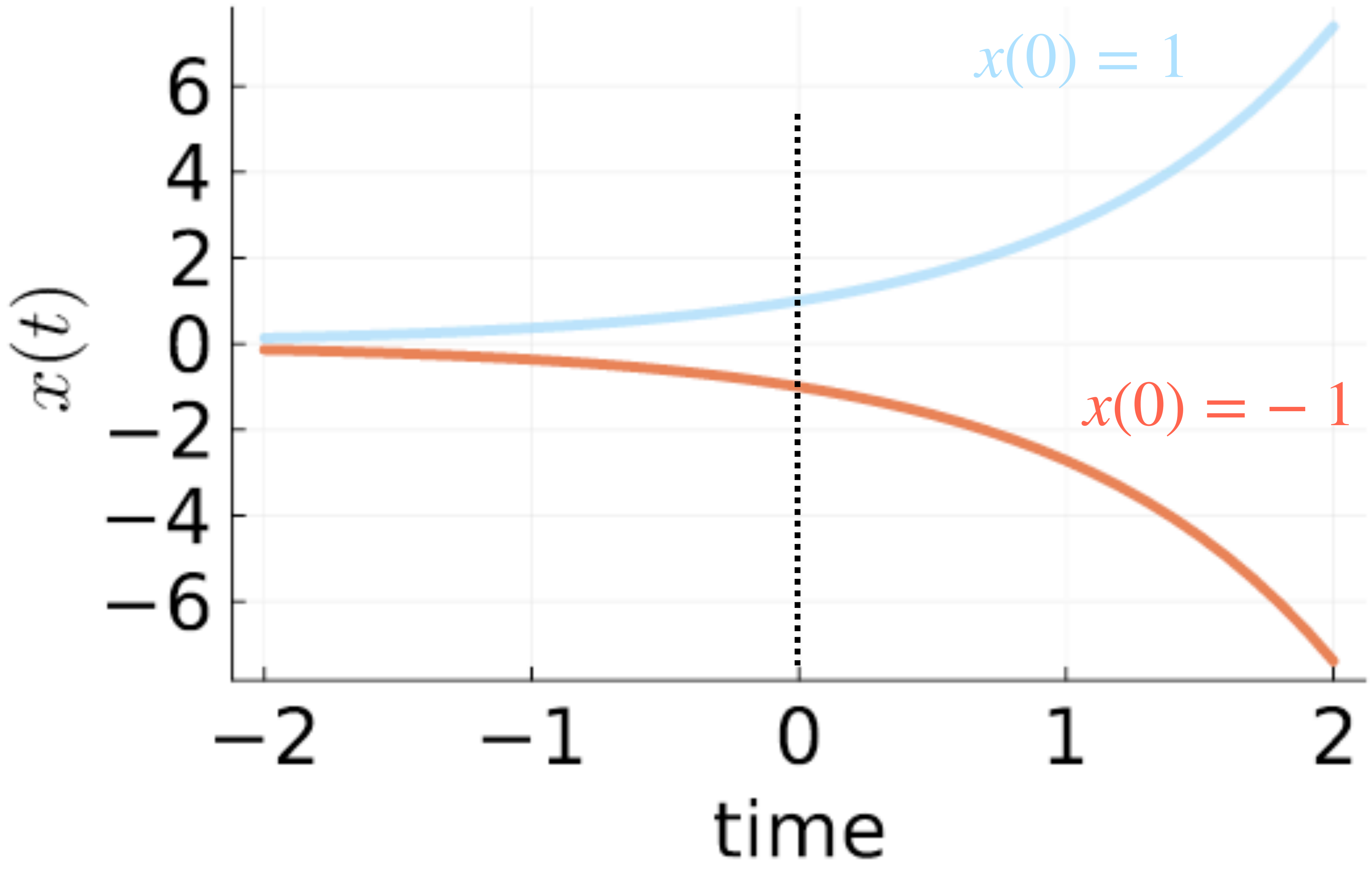
Evaluating numerical solvers

Will approximation error compound over time?



Evaluating numerical solvers

$$\dot{x}(t) = x(t)$$

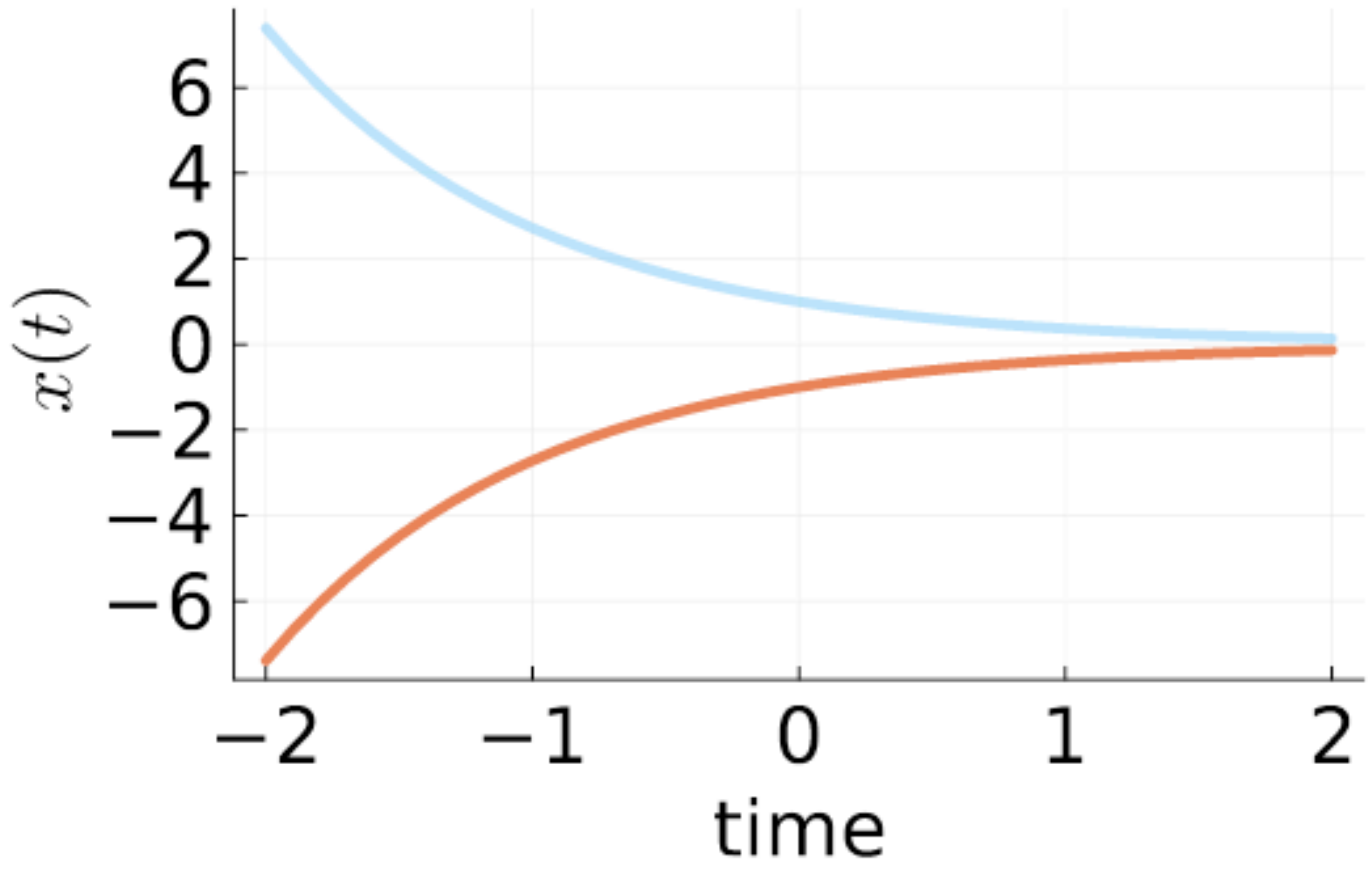


Will approximation error compound over time here?

Possibly! Small differences in true solution increase over time

Evaluating numerical solvers

$$\dot{x}(t) = -x(t)$$



Will approximation error compound over time here?

Less likely for this ODE?

Evaluating numerical solvers

When does approximation error compound over time?

Depends upon ODE, solving algorithm, initial conditions….

Mathematical analysis is hard. Difficult to explain intuition in lecture

Interactive seminar question instead

A good numerical solver should have….

Heuristics for stepsize δt that balance accuracy (small δt) with speed (large δt)

Small approximation error by cleverly interpolating information on $\dot{x}(t)$ over time steps

Warnings in situations where approximation error compounds

Numerical analysis is an entire field of mathematics

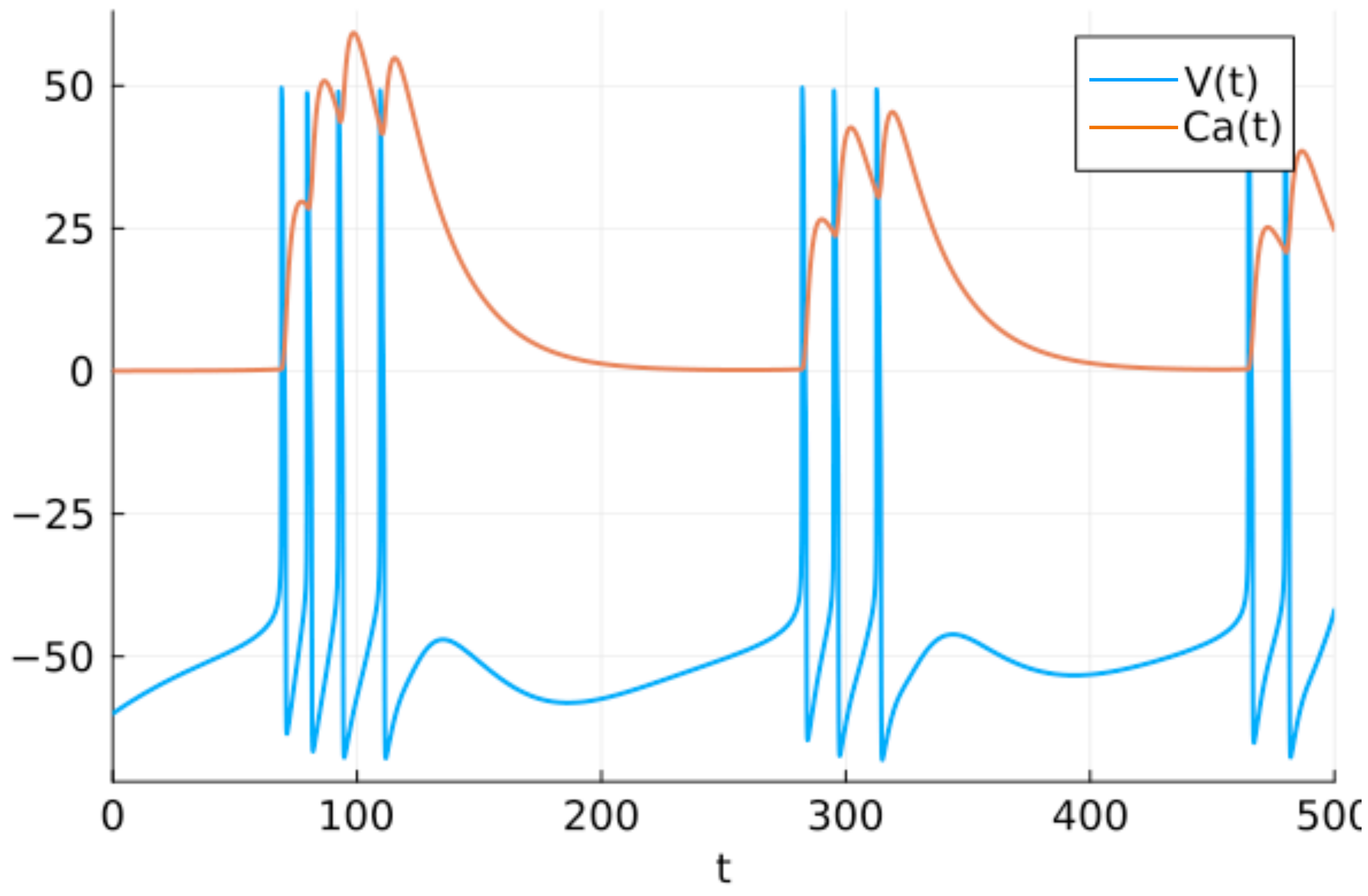
Stiff ODE example

Optimal δt changes drastically over time

Too big? Nonsense solution!

Specialised stiff ODE solvers exist

Voltage and calcium concentration in a bursting neuron model



No precise definition for stiffness

Solving first-order ODE in Python/Julia

```
scipy.integrate.solve_ivp
```

```
using OrdinaryDiffEq
solve(o::ODEProblem)
```

Choice of numerical solvers.
Picking the right one is an art!

(Scipy ones are slow, outdated and error-prone)

(Diffeqpy is a Julia port that does better)

Summary thus far

Gained some intuition on
how ODEs behave

Gained some intuition on numerical
solvers, and when they do badly

Haven't discussed how/why to model
real life processes with ODEs!….

Modelling (badly) a discrete stochastic dynamical system

N students. Every day, some of you get COVID…

Probability of infection per student on a given day: $\sim$ Bern(λ) (e.g. $\lambda = 0.1$)

S_i: number of healthy students on day i

Expected value of healthy students on a given day is easy to calculate

$$S_0 = N$$

$$\mathbb{E}[S_1] = (1 - \lambda)N$$

$$\mathbb{E}[S_2] = (1 - \lambda)^2 N$$

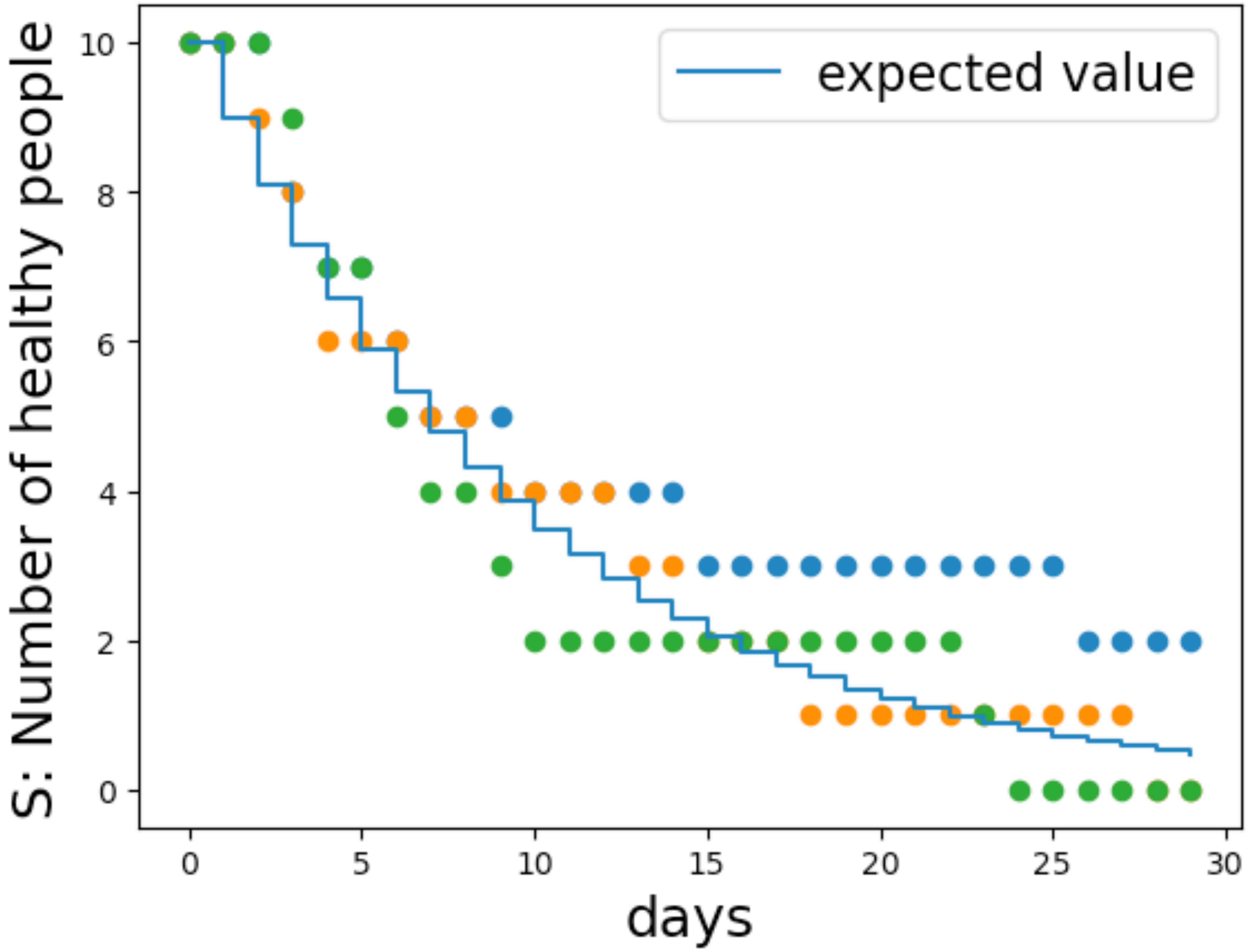
$$\vdots$$

$$\mathbb{E}[S_k] = (1 - \lambda)^k N$$

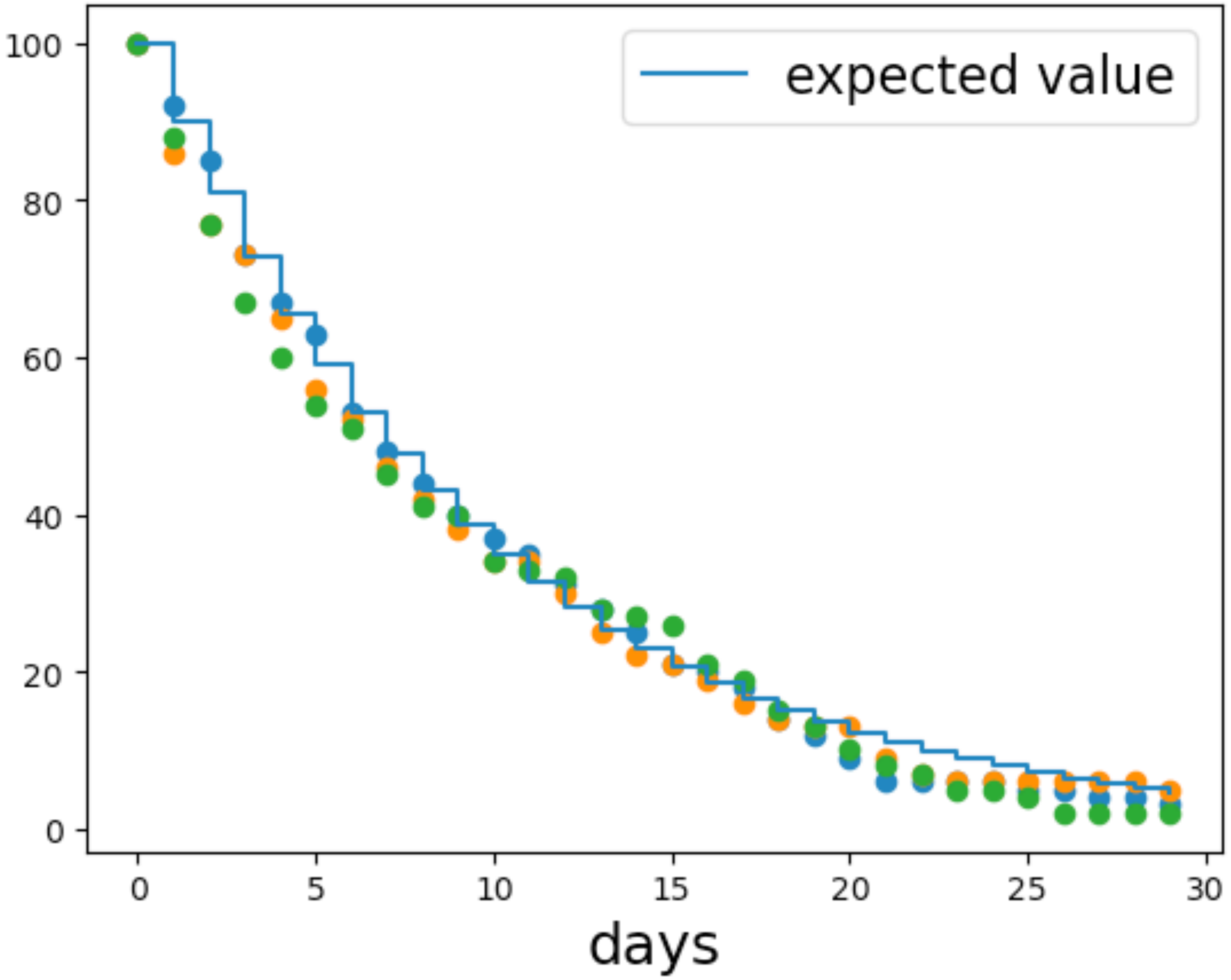
…but the variance is hard! Depends on previous days

If you can't calculate, simulate!

N=10, repeats = 4



N=100, repeats = 4



More students means less variance. Why?

What's wrong with our model?

Doesn't model many factors like recovery, changing immunity, etc.

- We'll get there!

Hard to analyse mathematically due to stochasticity

Infections don't actually occur on the stroke of midnight!

We’re going to approximate our model

Discrete time

t = 1 day, 2 days, …

Measure number of healthy people

Hard to analyse

Infections are stochastic

→

Continuous time ODE

Measure all timepoints

Measure expected number of healthy people

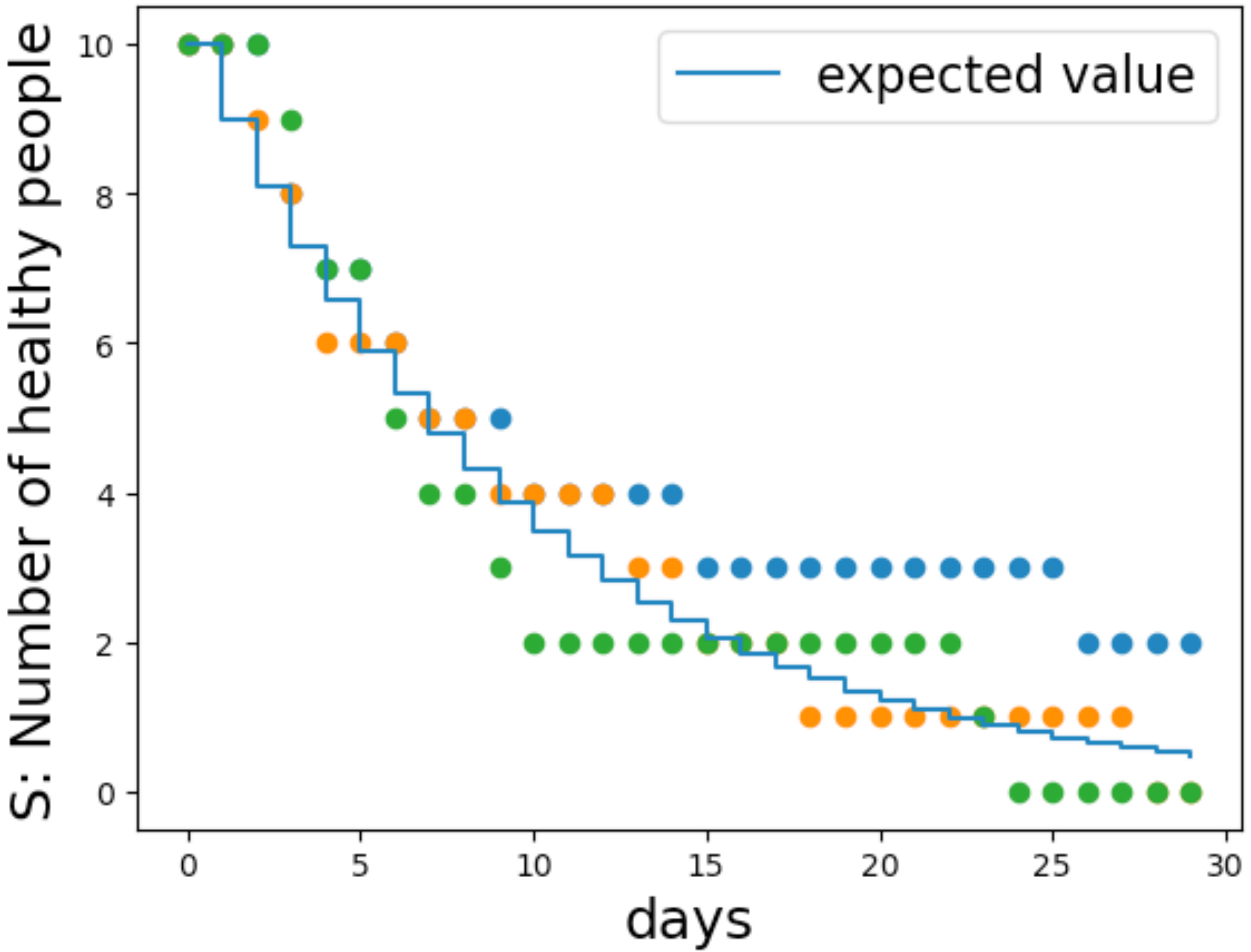
Easier to analyse

Only reasonable when stochasticity is low

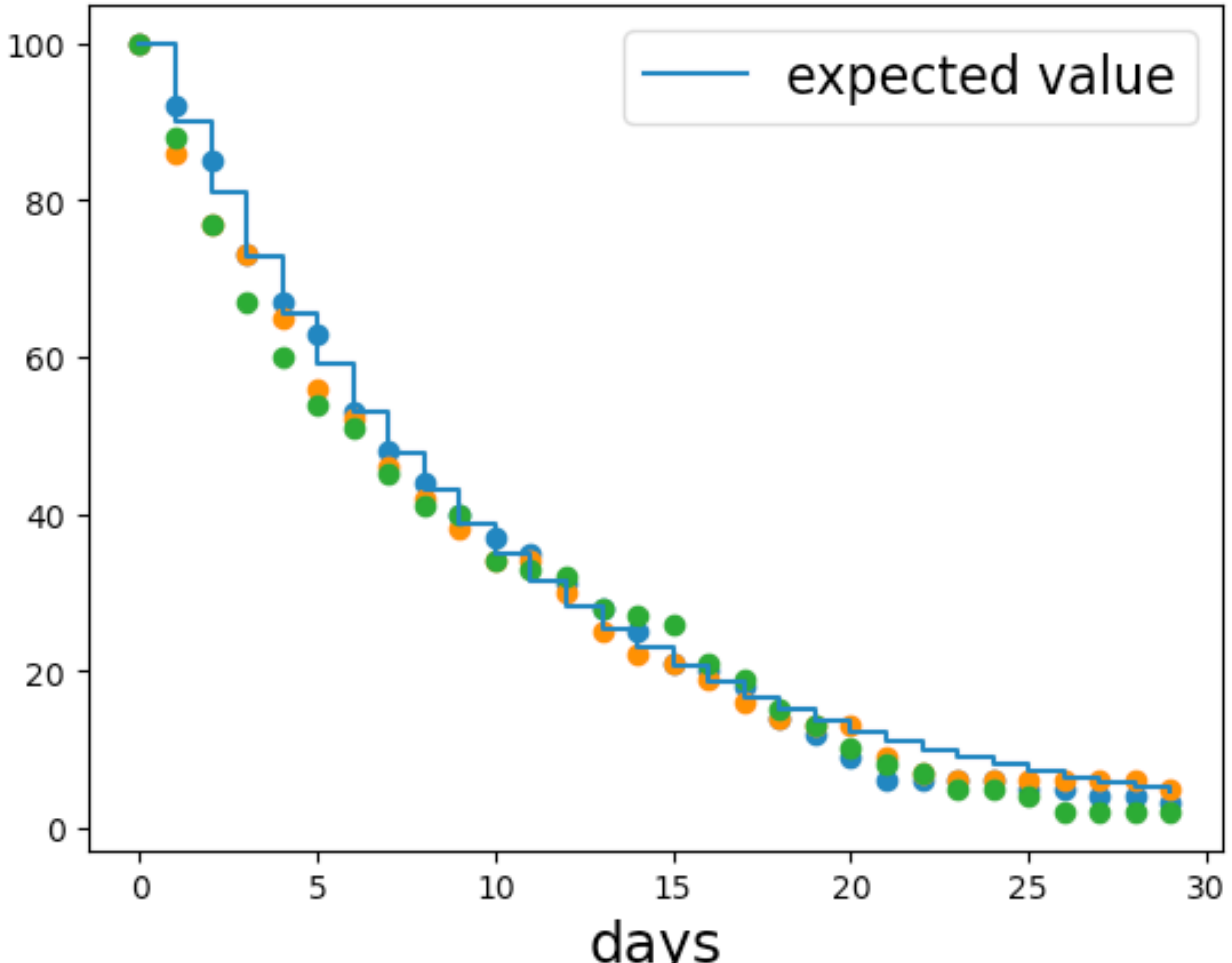
This is called a mean field approximation

It's how many ODE models are derived

Less valid (high stochasticity N=10)



Valid (low stochasticity, N=100)



Why are we only counting each day?

Infections can happen at any time.
Why not measure twice a day?

Current

$$S_{t+1} - S_t \sim - B(S_t, 1 - \lambda)$$

Measure twice a day

$$S_{t+\frac{1}{2}} - S_t \sim - B\left(S_t, \frac{1 - \lambda}{2}\right)$$

Why are we only counting each day?

Infections can happen at any time.
Why not measure at a timestep δt?

Current

$$S_{t+1} - S_t \sim -B(S_t, 1 - \lambda)$$

Measure every δt

$$S_{t+\delta t} - S_t \sim -B\left(S_t, \delta t(1 - \lambda)\right)$$

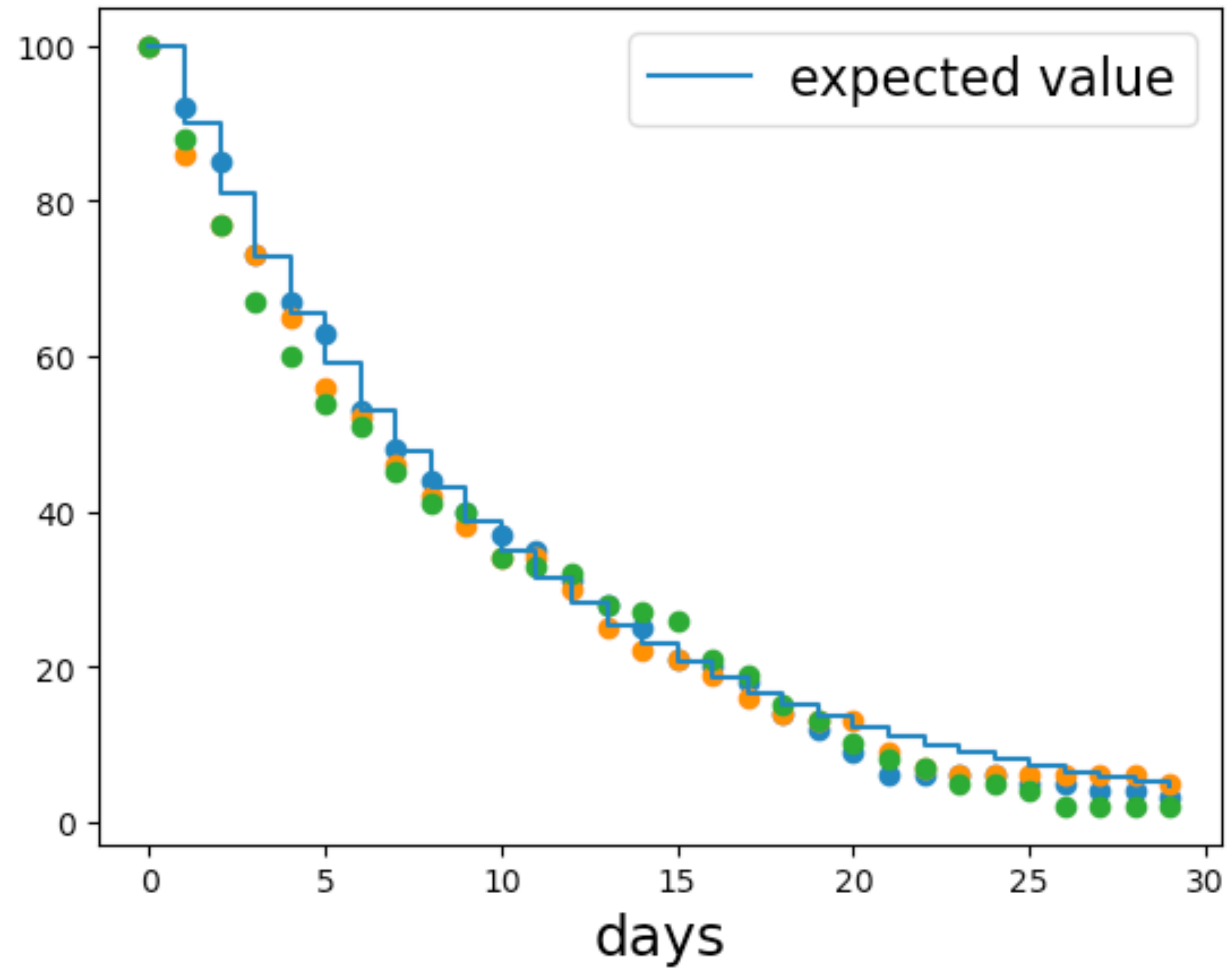
Measure twice a day

$$S_{t+\frac{1}{2}} - S_t \sim -B\left(S_t, \frac{1 - \lambda}{2}\right)$$

Hidden assumption

Expected number of infections is linear in time, for small time steps < 1 day

Clearly not true on longer timescales:



Questions for audience:

What's the source of the nonlinearity?

Why is short-timescale linearity reasonable?

Mean field equation for infection rate

Expected value of binomial: $$\mathbb{E}[S_{t+\delta t} - S_t] = -S_t \delta t (1-\lambda)$$

Rearranging and removing expectations for clarity: $$\frac{S_{t+\delta t} - S_t}{\delta t} = -pS_t \qquad p = (1-\lambda)$$

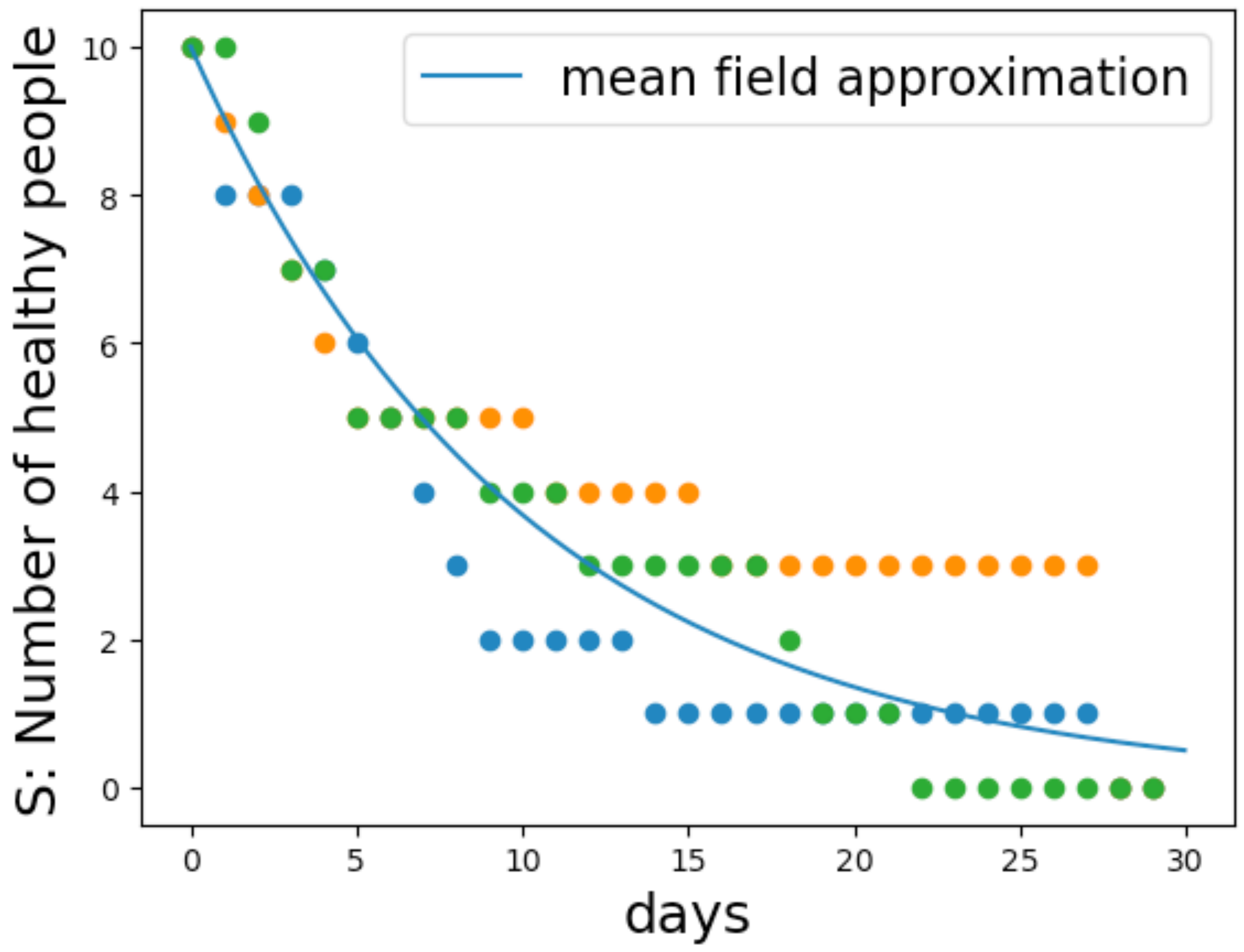
Limit as $\delta t \to 0$ $$\boxed{\dot{S}(t) = -pS(t)}$$

What have we done?

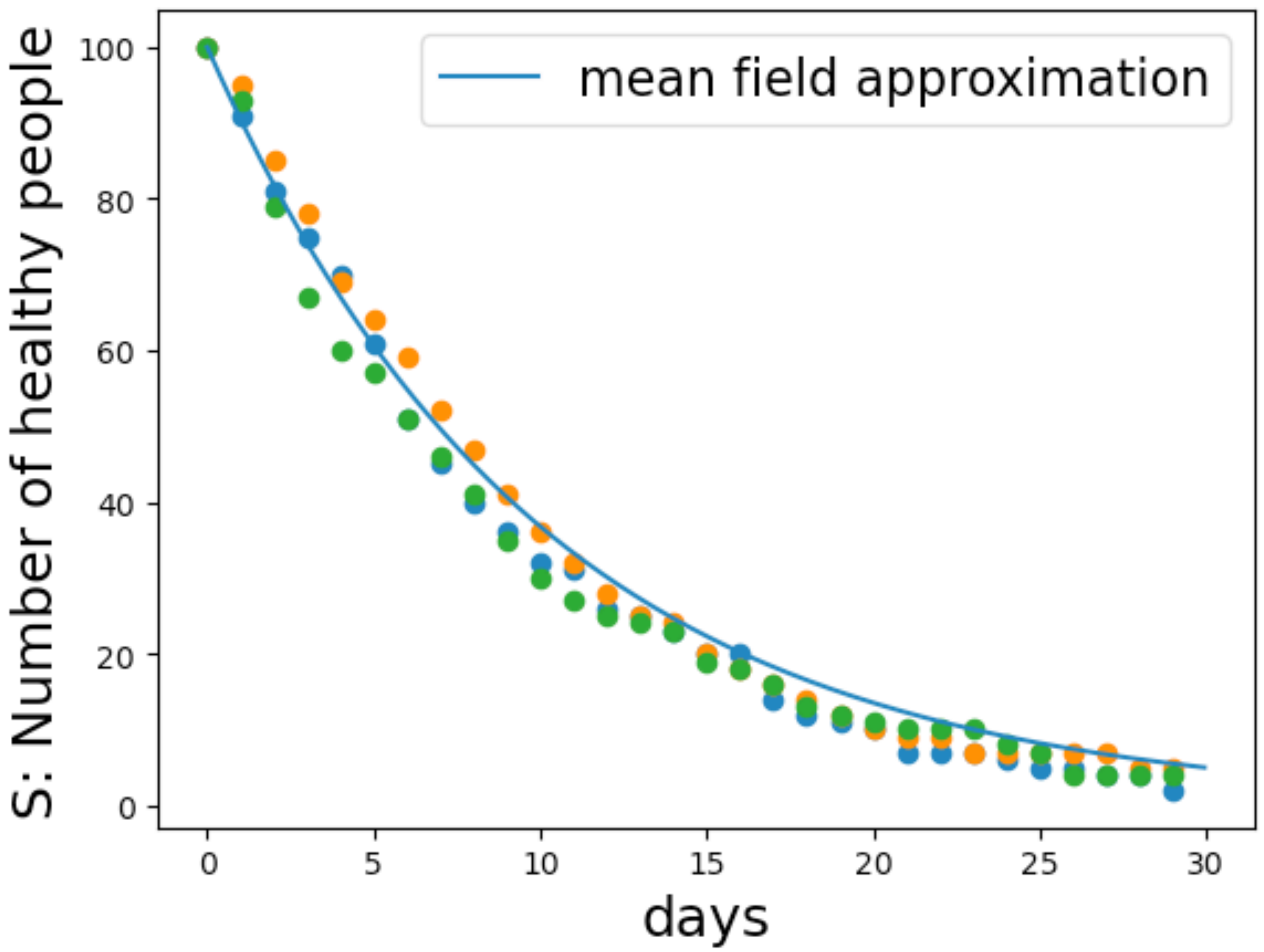
Rewritten what we expect a stochastic process to do as an ODE

$$\boxed{\dot{S}(t) = -pS(t)}$$

N=10



N=100



Analytical solution is easy in this case

$$\boxed{\begin{aligned}\dot{S}(t) &= -pS(t)\\ S(0) &= N\end{aligned}} \quad \Rightarrow \quad S(t) = N\exp(-pt)$$

Solve for yourself. Use previous analytical solution to help

Interpreting our (bad) model

$$\dot{S}(t) = -pS(t)$$
$$S(0) = N$$

What are the units of p?

(Units on each side of equation should be equal)

Interpreting our (bad) model

$$\frac{\mathrm{d}S}{\mathrm{d}t}(t) = -pS(t)$$

$$\frac{\text{Number}}{\text{time}} = \text{Units of p} \times \text{Number}$$

$$\boxed{\text{Units of } p \text{ are } \frac{1}{\text{time}}}$$

p is a rate (the intrinsic infection rate)

What’s wrong with our model?

Doesn’t model many factors like recovery, changing immunity, etc.

Hard to analyse mathematically due to stochasticity

- Sorted!

Infections don’t occur on the stroke of midnight!

- Sorted!

Systems of ODEs

Single state represented as number
(e.g. number of healthy students)

Previously

$$\dot{x}(t) = f\big((x(t), t\big)$$

Multiple interacting states
represented as vector

Next

$$\dot{x}(t) = f\big((x(t), t\big)$$

ODEs useful for analysing dynamic interactions
between quantities

SI Model

Mean dynamics of healthy students
(from before)

$$\dot{S}(t) = -pS(t)$$
$$S(0) = N$$

Dynamics of infected students?

$$\dot{I}(t) = ???$$
$$I(0) = 0$$

SI Model

Total students doesn't change
(no deaths)

$$\forall t : S(t) + I(t) = N$$

Differentiating in time:

$$\dot{S}(t) + \dot{I}(t) = 0$$

$$\Rightarrow \dot{I}(t) = -\dot{S}(t)$$

SI Model

New model:

$$\begin{bmatrix} \dot{S}(t) \\ \dot{I}(t) \end{bmatrix} = \begin{bmatrix} -p & 0 \\ p & 0 \end{bmatrix} \begin{bmatrix} S(t) \\ I(t) \end{bmatrix}$$

$$\dot{x}(t) = Ax(t)$$

$$\begin{bmatrix} S(0) \\ I(0) \end{bmatrix} = \begin{bmatrix} N \\ 0 \end{bmatrix}$$

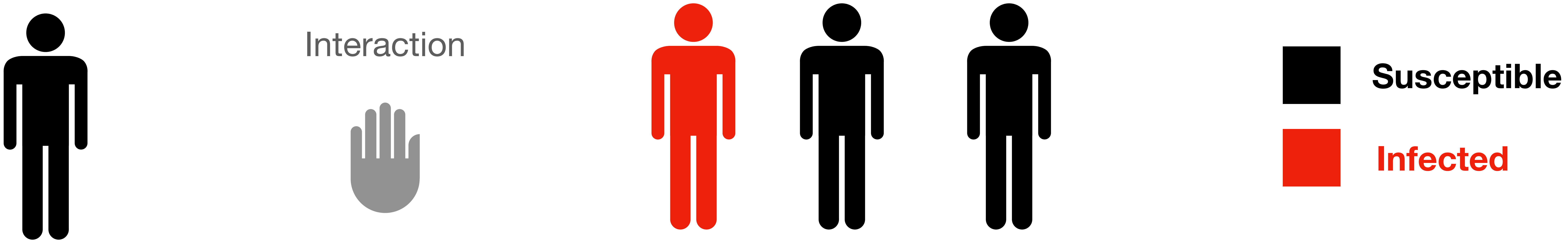
$$x(0) = \begin{bmatrix} S(0) \\ I(0) \end{bmatrix}$$

…still a linear first-order ODE!

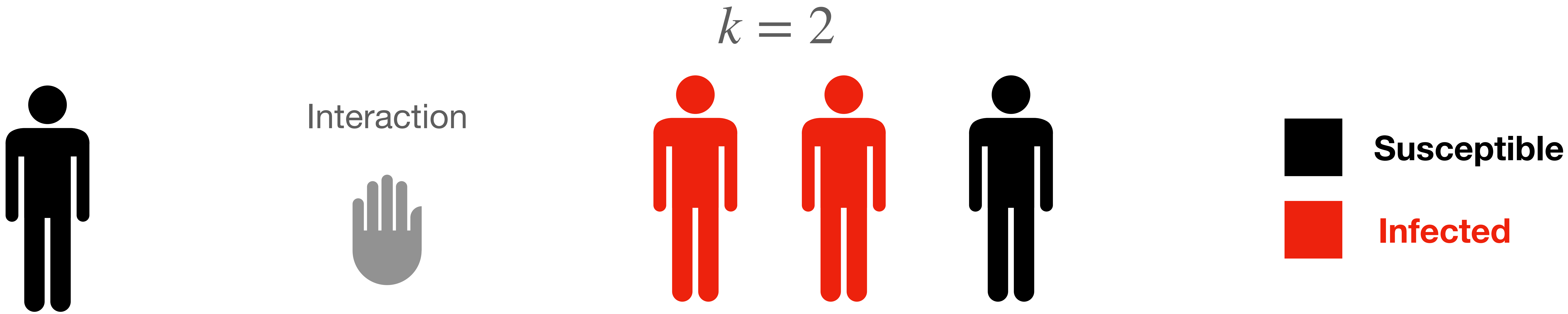
Improving the SI model

Overall rate of infection should depend on
number of susceptibles and number of infected

But how?



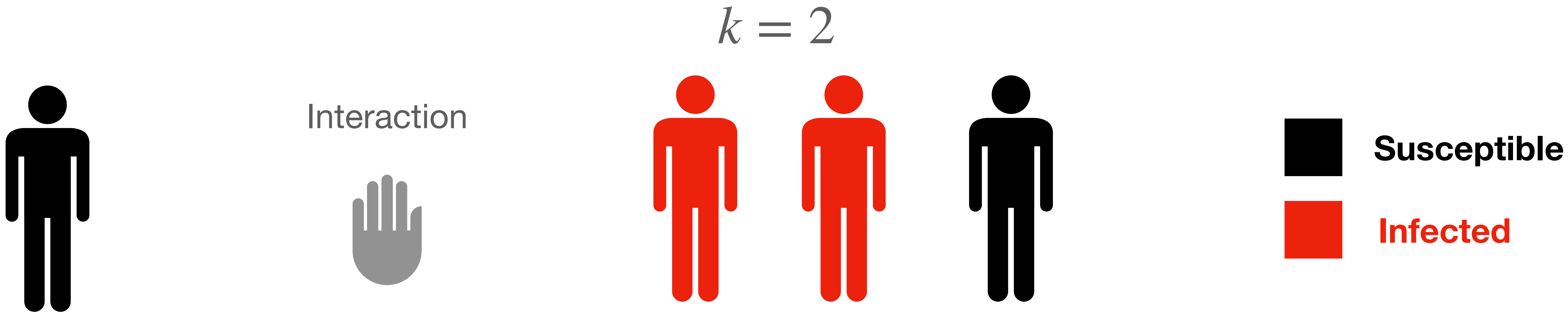
Improving the SI model



Increase proportion of infected individuals by factor of k

Increase infection rate by factor of k

Improving the SI model

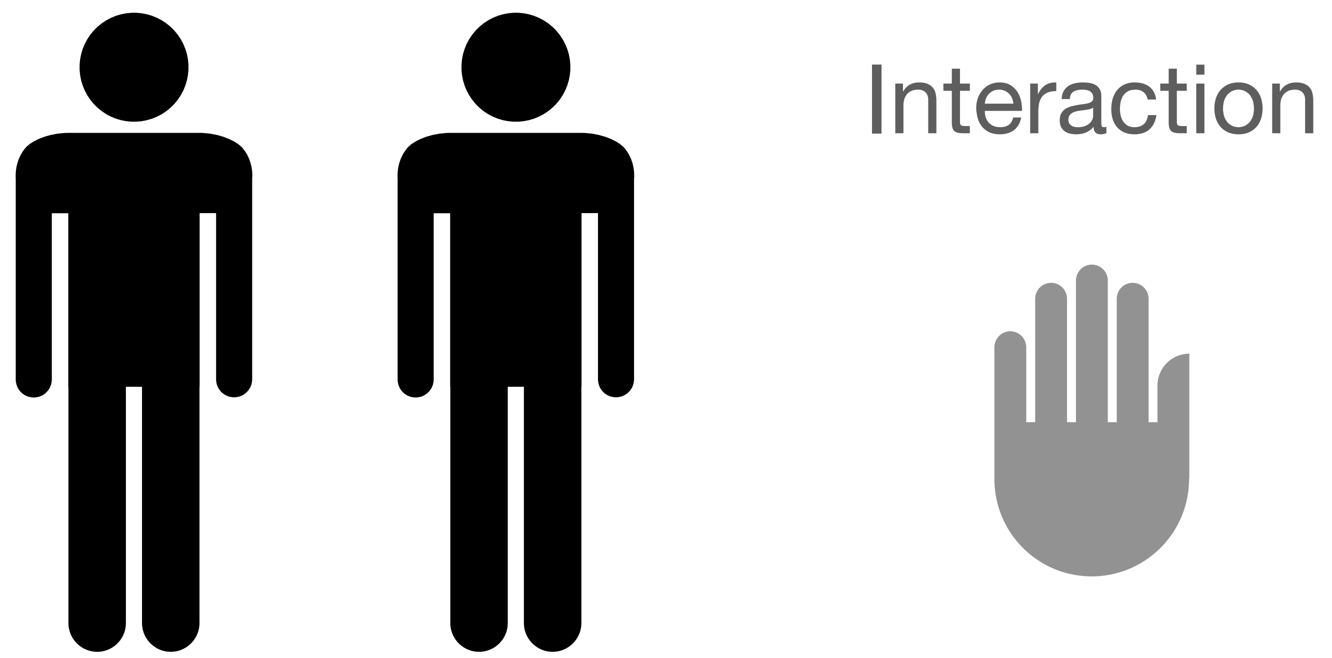


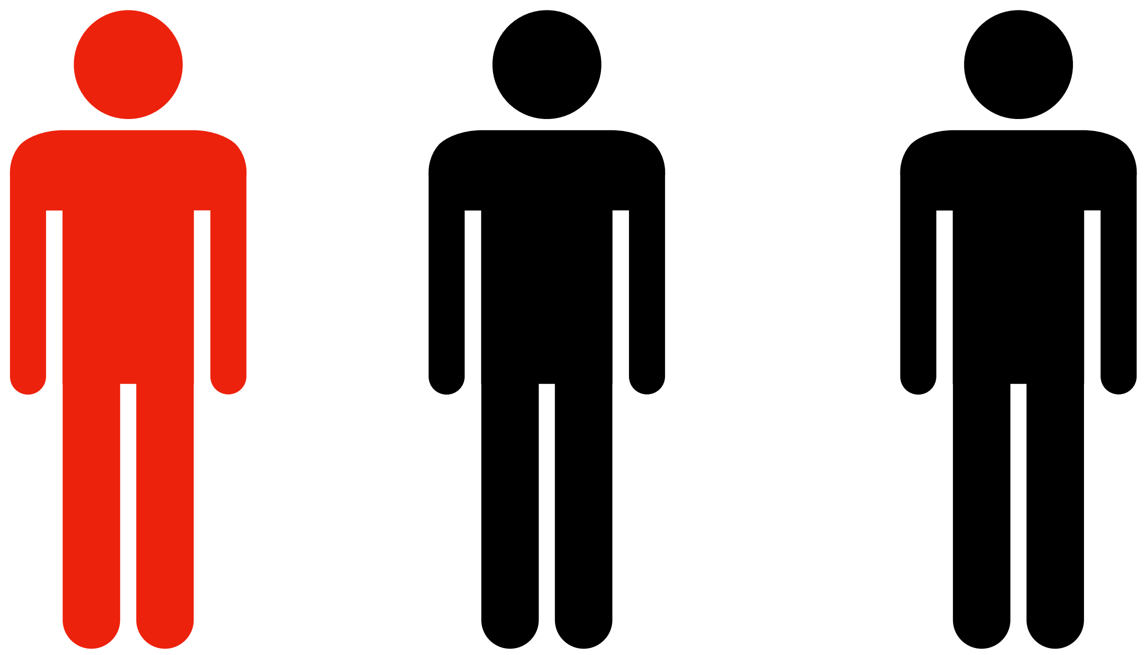
Increase proportion of infected individuals by factor of k → Increase infection rate by factor of k

$$\dot{S}(t) \propto -p\frac{I(t)}{N}$$

Improving the SI model

$k = 2$





Increase susceptible individuals by factor of k

Increase infection rate by factor of k

Improving the SI model

$$\boxed{\dot{S}(t) \propto -\frac{pS(t)I(t)}{N}}$$

Note

Could have $\tilde{p} = \frac{p}{N}$, but nice to have population-independent measure of infectivity

Improved SI Model

$$\dot{S}(t) = -p\frac{S(t)I(t)}{N}$$

$$\dot{I}(t) = \quad p\frac{S(t)I(t)}{N}$$

$$\begin{bmatrix} S(0) \\ I(0) \end{bmatrix} = \begin{bmatrix} N \\ 0 \end{bmatrix}$$

Now it's nonlinear :(

Improving the SI model

Every infectious person
eventually recovers (no deaths)

Same type of stochastic
process as infection

Same mean field
approximation

The standard SIR model

$$\dot{S}(t) = -p\frac{S(t)I(t)}{N}$$

$$\dot{I}(t) = p\frac{S(t)I(t)}{N} - \gamma I(t)$$

$$\dot{R}(t) = \gamma I(t)$$

p: infection rate

γ: recovery rate

$$\dot{S}(t) + \dot{I}(t) + \dot{R}(t)?$$

The standard SIR model

p: infection rate

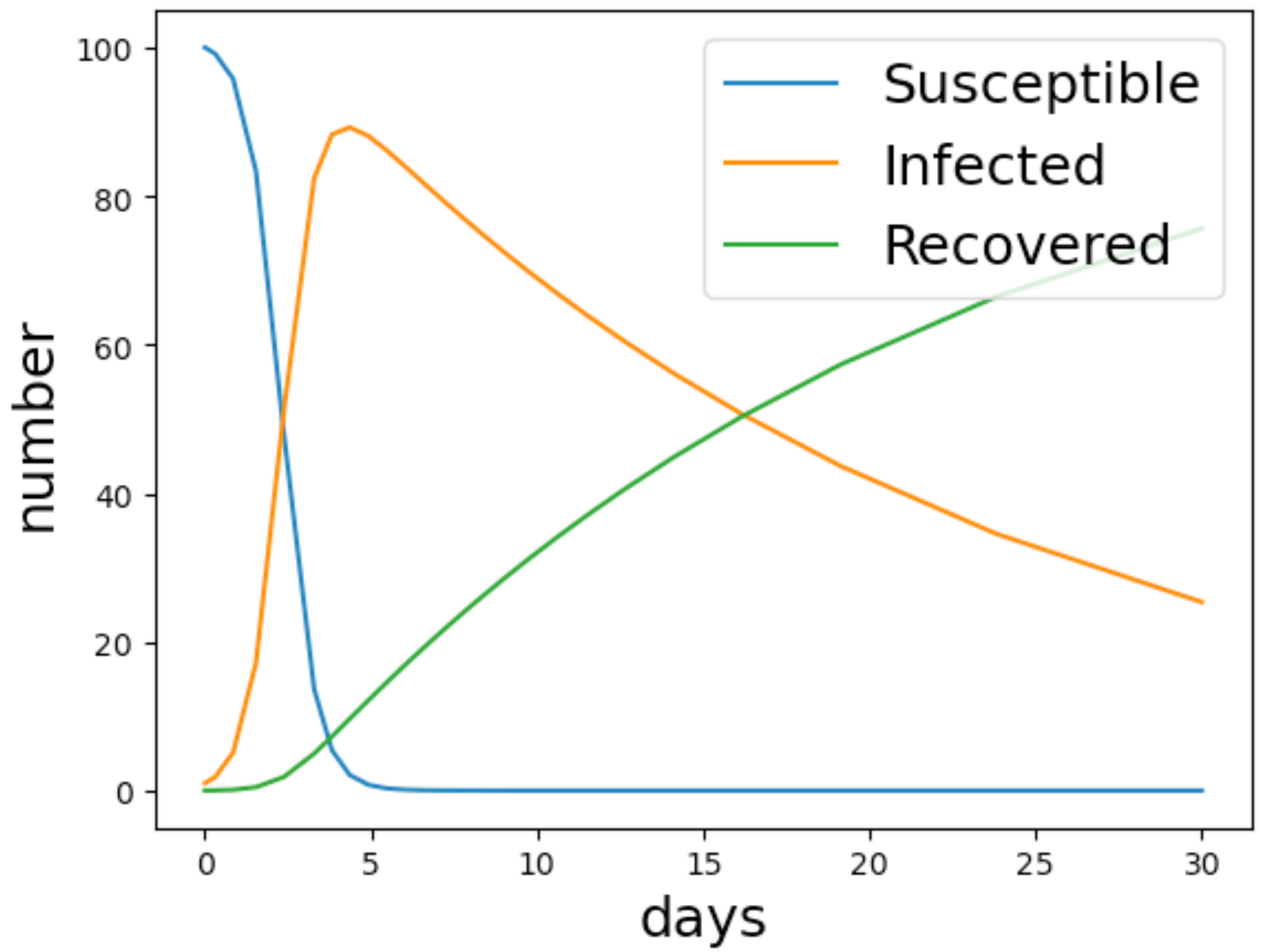
γ: recovery rate

$$\begin{aligned}
\dot{S}(t) &= -p\frac{S(t)I(t)}{N} \\
\dot{I}(t) &= p\frac{S(t)I(t)}{N} - \gamma I(t) \\
\dot{R}(t) &= \gamma I(t)
\end{aligned}$$

$$\Downarrow$$

$$x(t) = \begin{bmatrix} S \\ I \\ R \end{bmatrix} \qquad \dot{x}(t) = f(x(t), t)$$

Plotting the SIR model



$$\dot{S}(t) = -p\frac{S(t)I(t)}{N}$$

$$\dot{I}(t) = p\frac{S(t)I(t)}{N} - \gamma I(t)$$

$$\dot{R}(t) = \gamma I(t)$$

Experienced modeller can intuit shape of graph from equations, without simulating

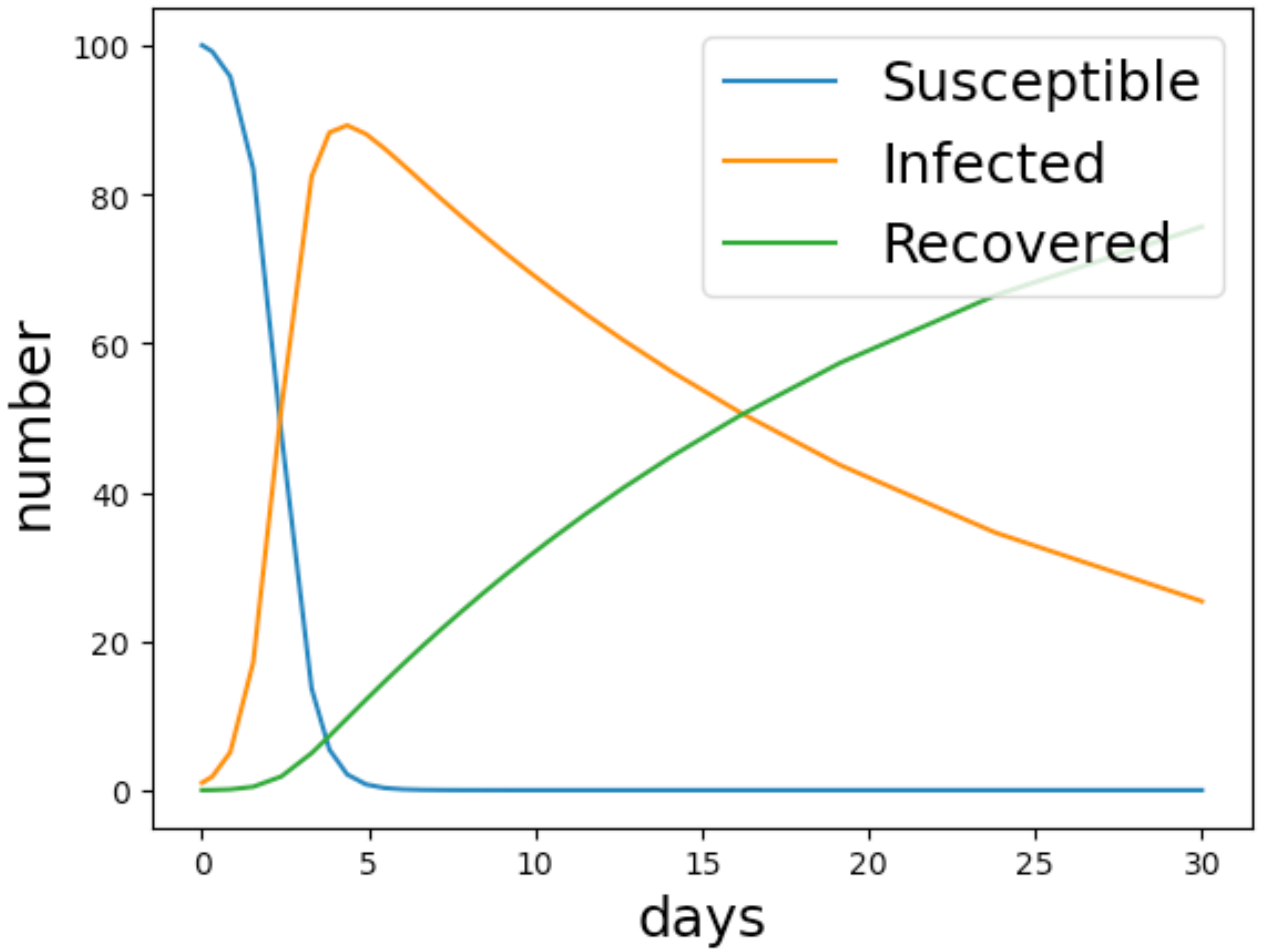
Analysis

Dynamics depend upon
parameters

$$\dot{S}(t) = -\frac{p}{N}S(t)I(t)$$

$$\dot{I}(t) = \frac{p}{N}S(t)I(t) - \gamma I(t)$$

$$\dot{R}(t) = \gamma I(t)$$



What combination of parameters could avoid a pandemic?

Need expected infections to always be decreasing

Analysis

$$\dot{S}(t) = -\frac{p}{N}S(t)I(t)$$

$$\dot{I}(t) = \frac{p}{N}S(t)I(t) - \gamma I(t)$$

$$\dot{R}(t) = \gamma I(t)$$

Dynamics depend upon parameters

What combination of parameters could avoid a pandemic?

Need expected infections to always be decreasing

$$\dot{I}(0) < 0 \quad \Rightarrow \frac{p}{N}N - \gamma < 0$$

$$\Rightarrow \frac{p}{\gamma} < 1$$

The basic reproduction number

$$R_0 = \frac{p}{\gamma}$$

$R_0 < 1$: a single infected person in the population will infect less than one person, on average

Question for the audience

$$R_0 = \frac{p}{\gamma}$$

How would you model vaccination?
Social distancing?

Can you comment on herd immunity
in the context of this model?

Herd immunity

$$R_0 = \frac{p}{\gamma}$$

How would you model vaccination? Social distancing?

Could add extra state for the vaccinated. Or just decrease p

Can you comment on herd immunity in the context of this model?

Vaccination/distancing need only decrease infectivity until $R_0 < 1$.

Fixed points of the SIR model

p: infection rate

γ: recovery rate

$$\dot{S}(t) = -p\frac{S(t)I(t)}{N}$$

$$\dot{I}(t) = \left(p\frac{S(t)}{N} - \gamma\right)I(t)$$

$$\dot{R}(t) = \gamma I(t)$$

For what values of S, I, R are there no dynamics?

Steady state analysis of SIR model

$$\dot{S}(t) = -p\frac{S(t)I(t)}{N}$$

$$\dot{I}(t) = \left(p\frac{S(t)}{N} - \gamma\right)I(t)$$

$$\dot{R}(t) = \gamma I(t)$$

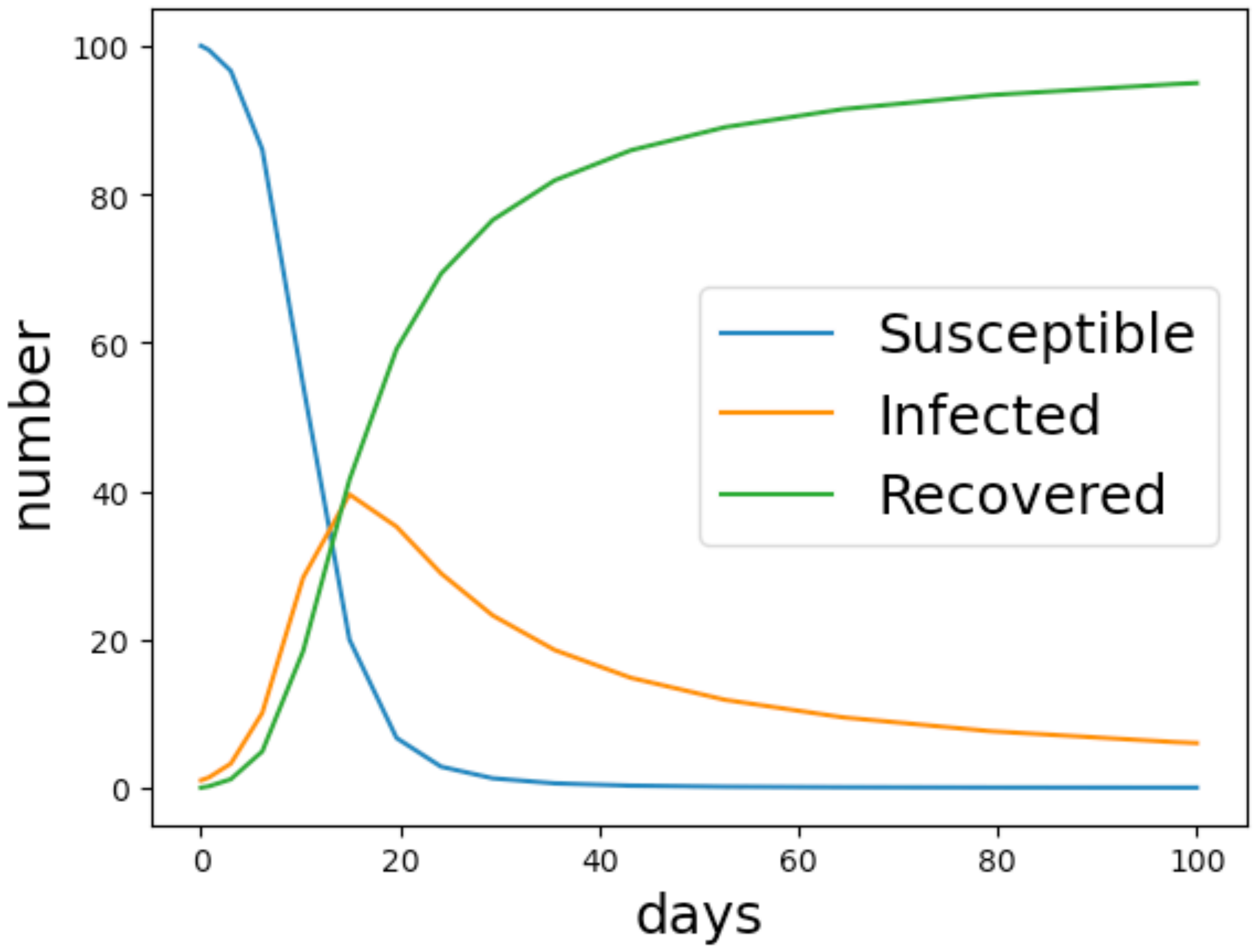
Fixed point: $I(t) = 0$.
$S(t), R(t)$ can be anything!

But not all fixed points are created equal!…

Deviation from a fixed point

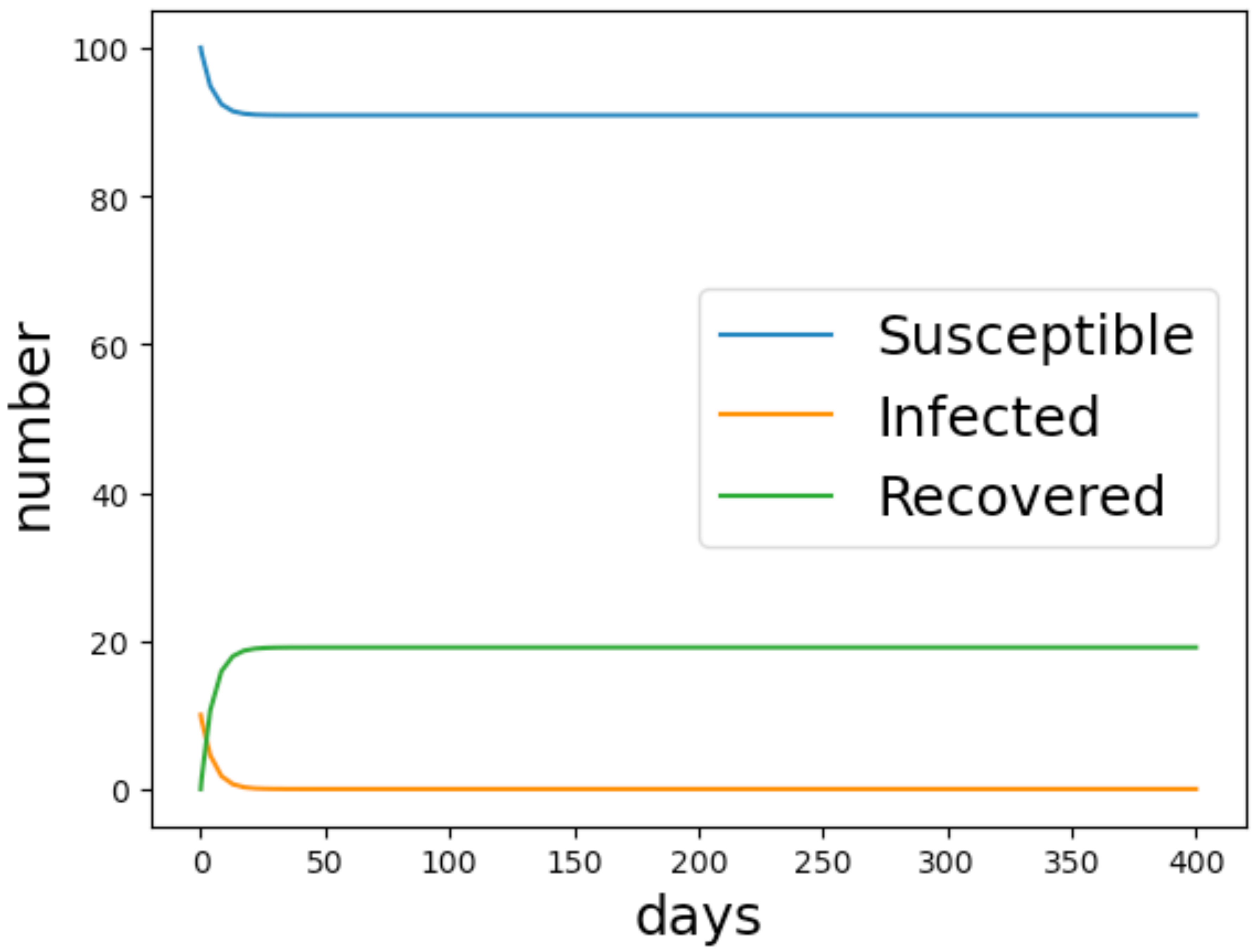
add a single infection…

$R_0 > 1$



Unstable: infections increase away from the fixed point. Pandemic!

$R_0 < 1$



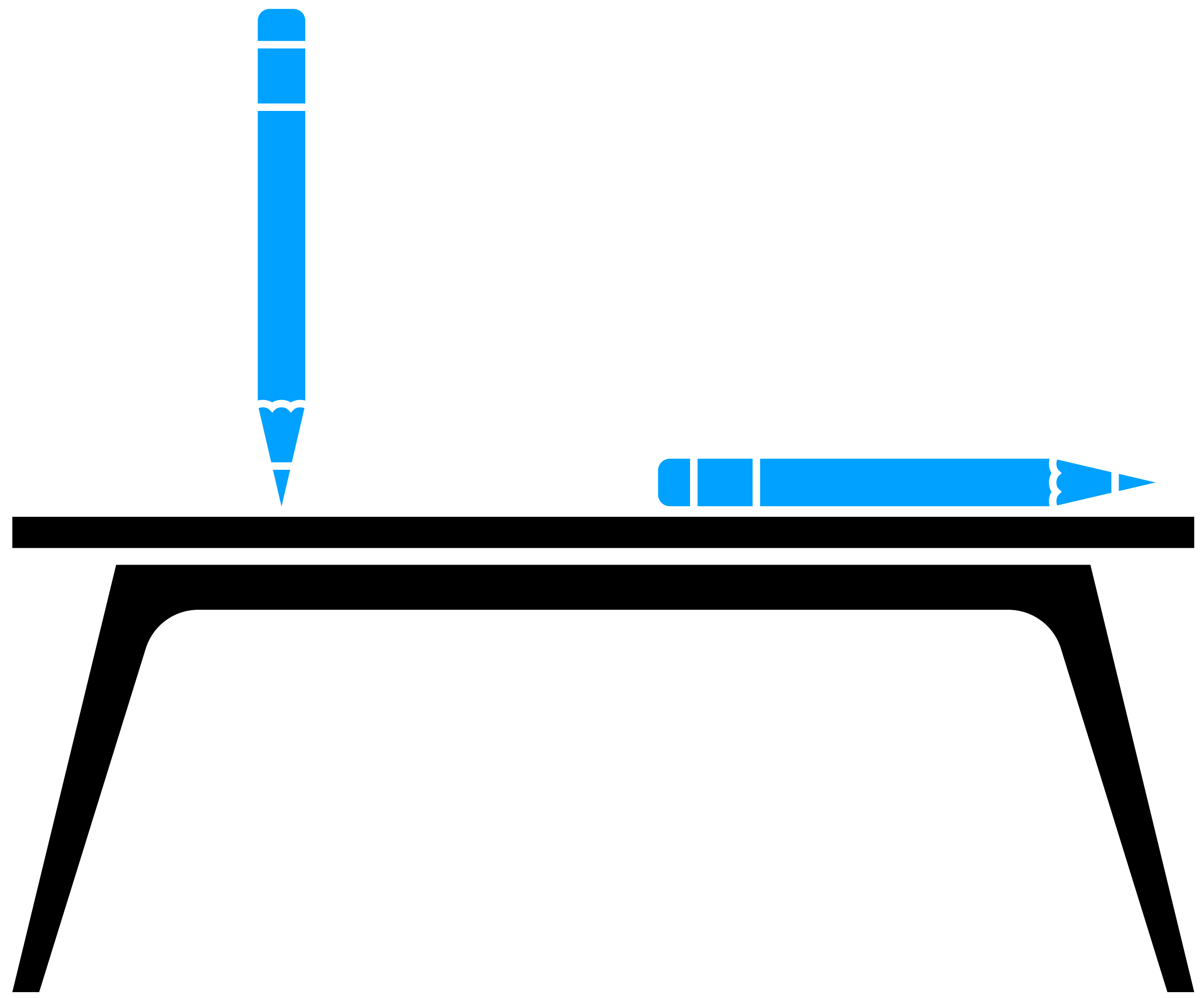
Stable: infections decrease back to the fixed point

Fixed points for general ODE

$$\dot{x}(t) = f(x(t), t)$$
$$\dot{x}(0) = x_0$$

Fixed points:

$$\boxed{\{x^* : f(x^*, t) = 0\}}$$



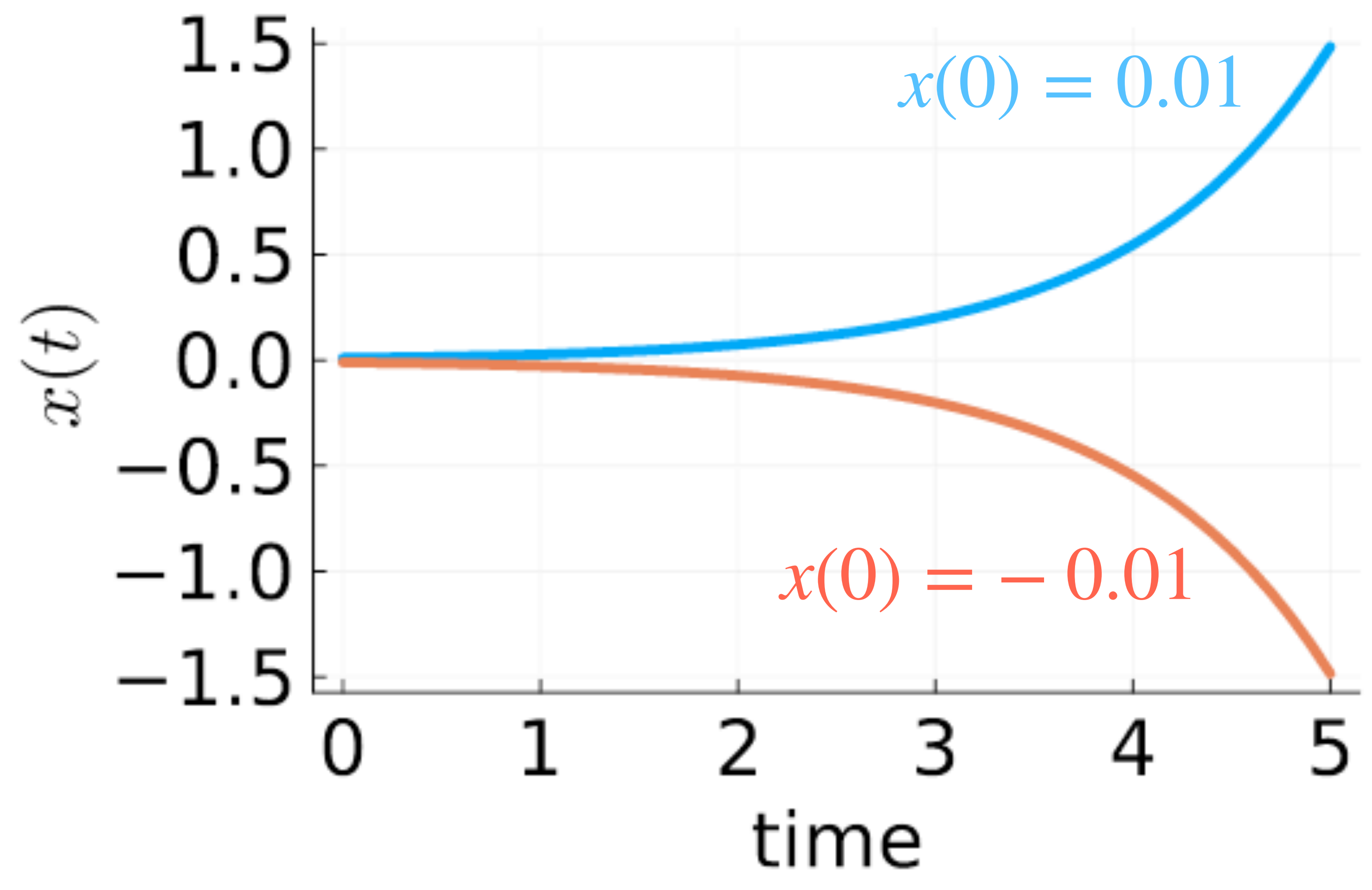
Definition of stability?

Can we infer from equations without simulating?

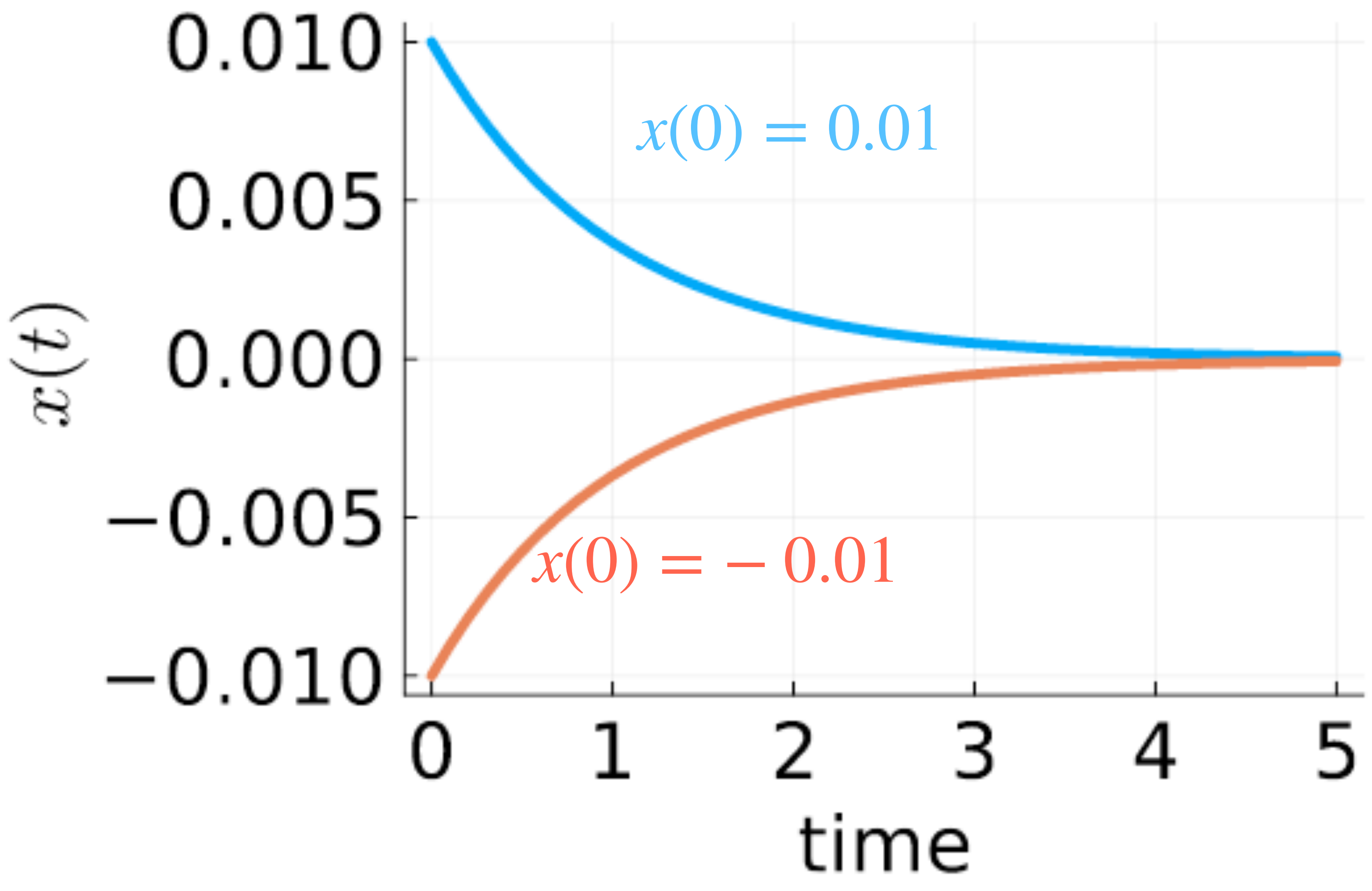
Fixed points for scalar ODE

Small fixed point deviations with different effects:

$$\dot{x}(t) = x(t)$$

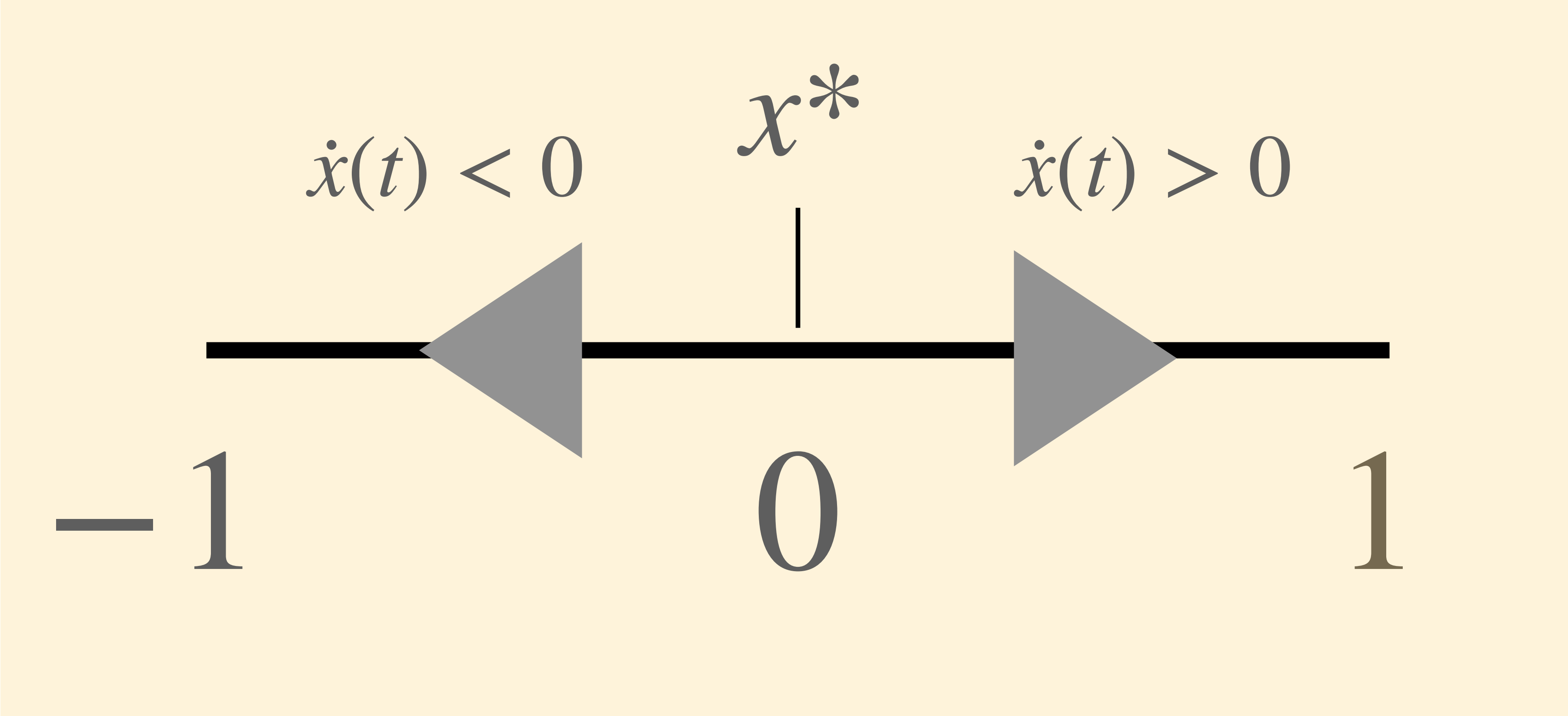


$$\dot{x}(t) = -x(t)$$



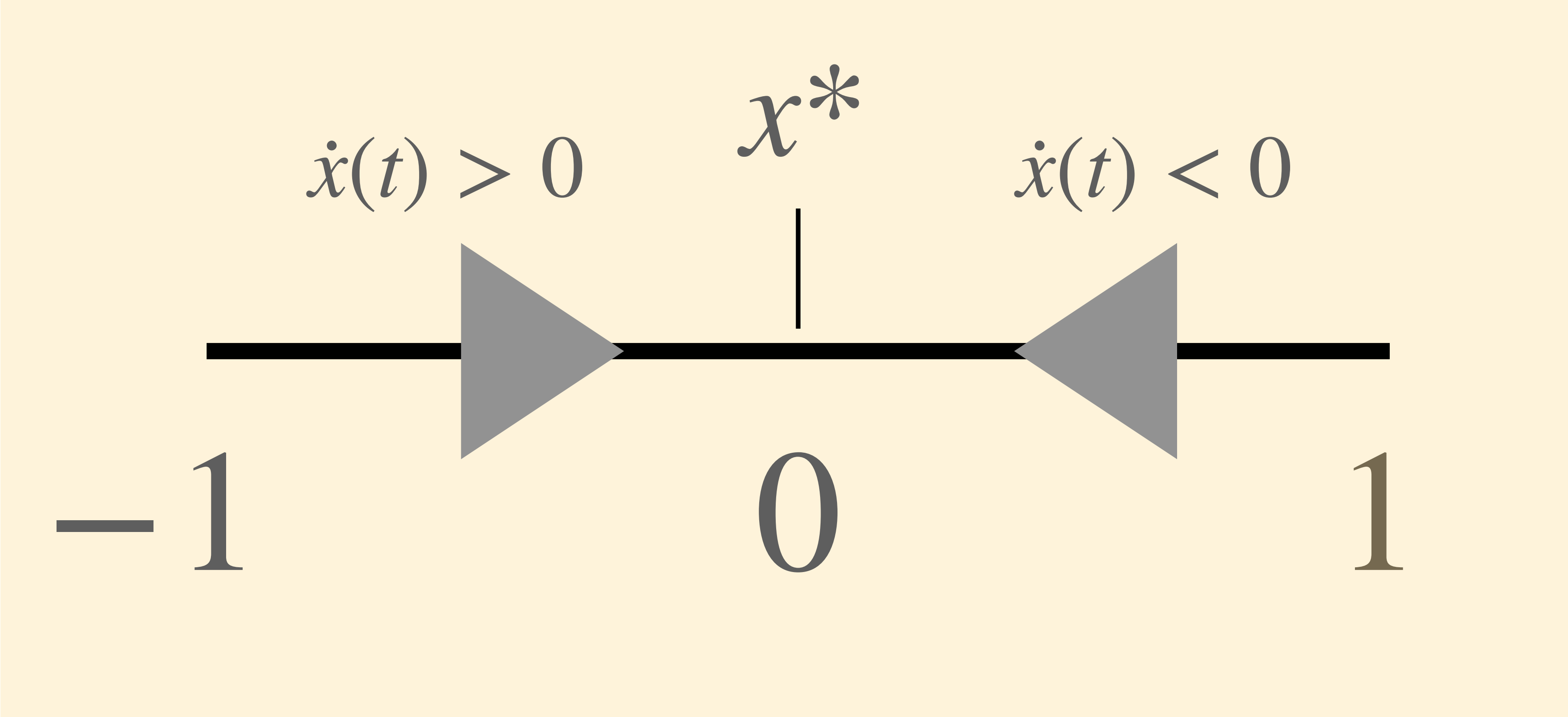
Fixed points for scalar ODE

$$\dot{x}(t) = x(t)$$



Perturbation travels away from fixed point

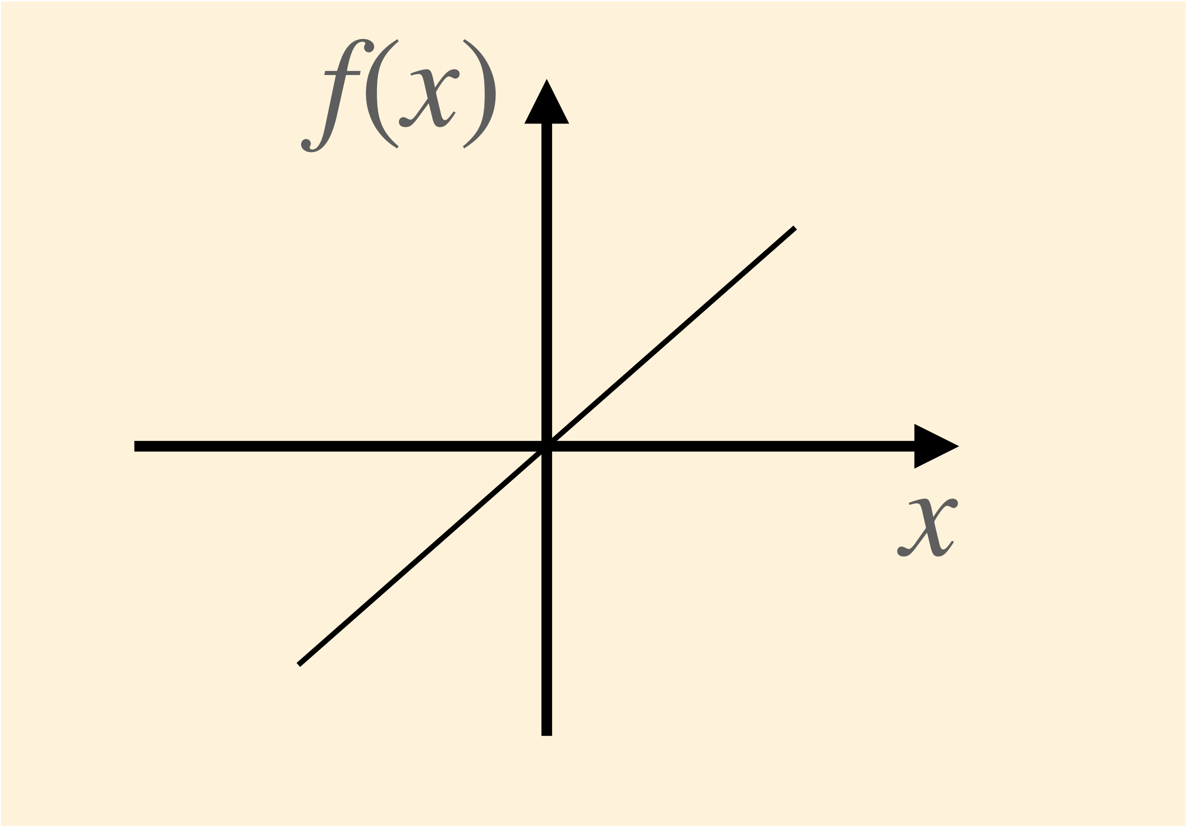
$$\dot{x}(t) = -x(t)$$



Perturbation travels back into fixed point

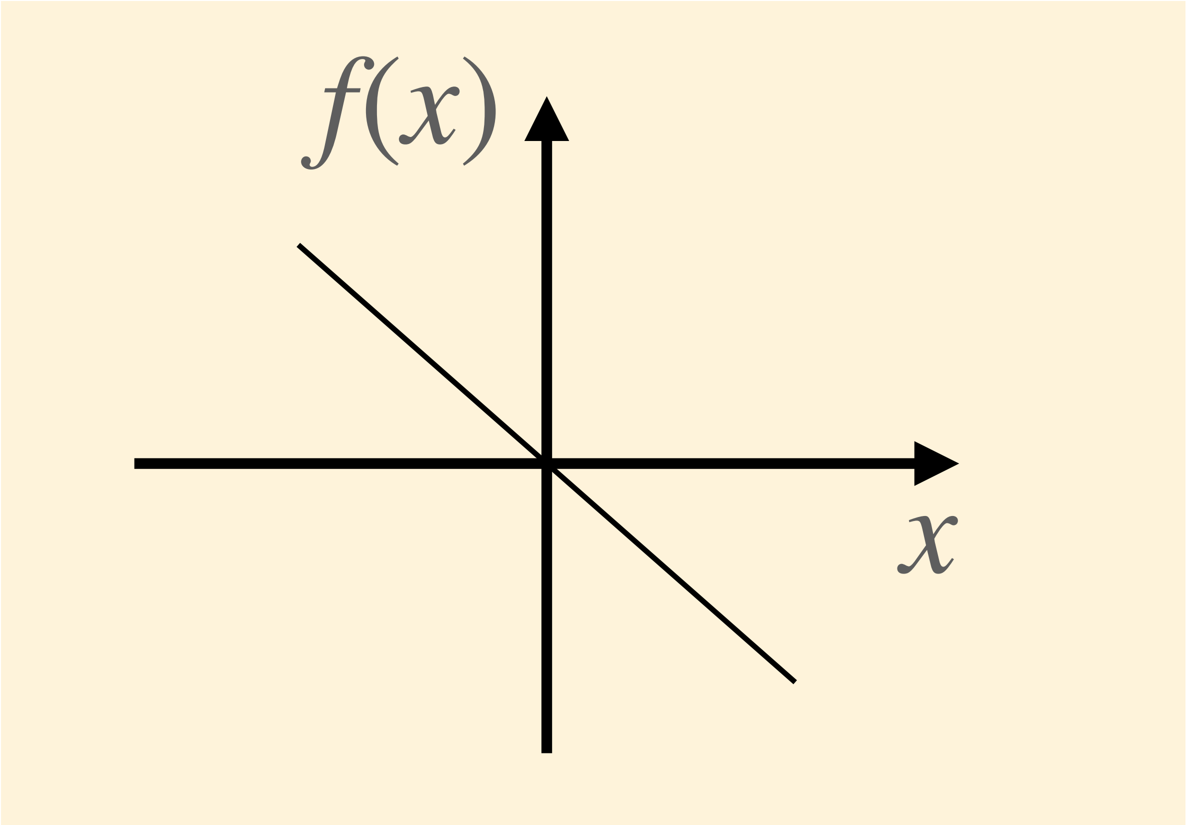
Fixed points for scalar ODE $\dot{x}(t) = f\big(x(t)\big)$

$$\dot{x}(t) = x(t)$$



$$\frac{\partial f}{\partial x} = 1 > 0$$

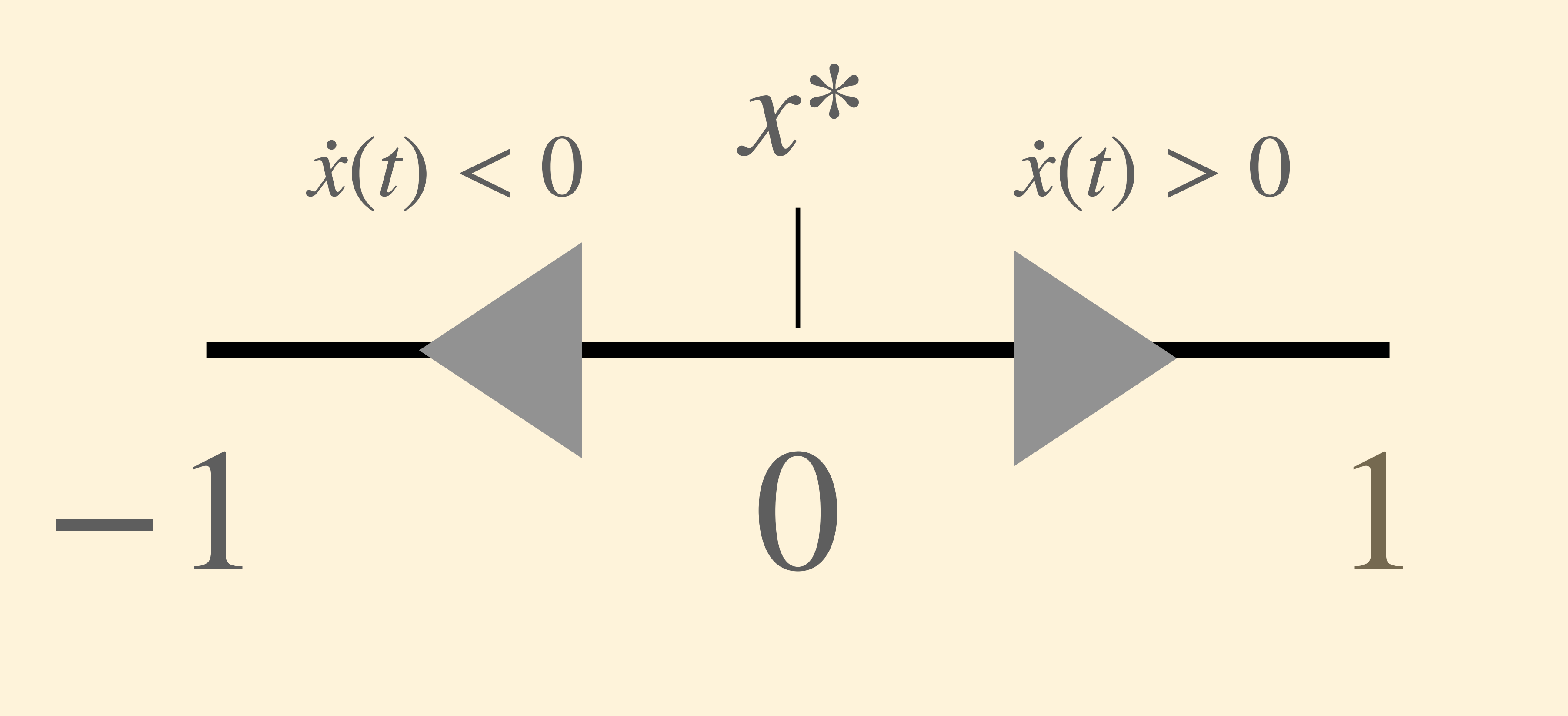
$$\dot{x}(t) = -x(t)$$



$$\frac{\partial f}{\partial x} = -1 < 0$$

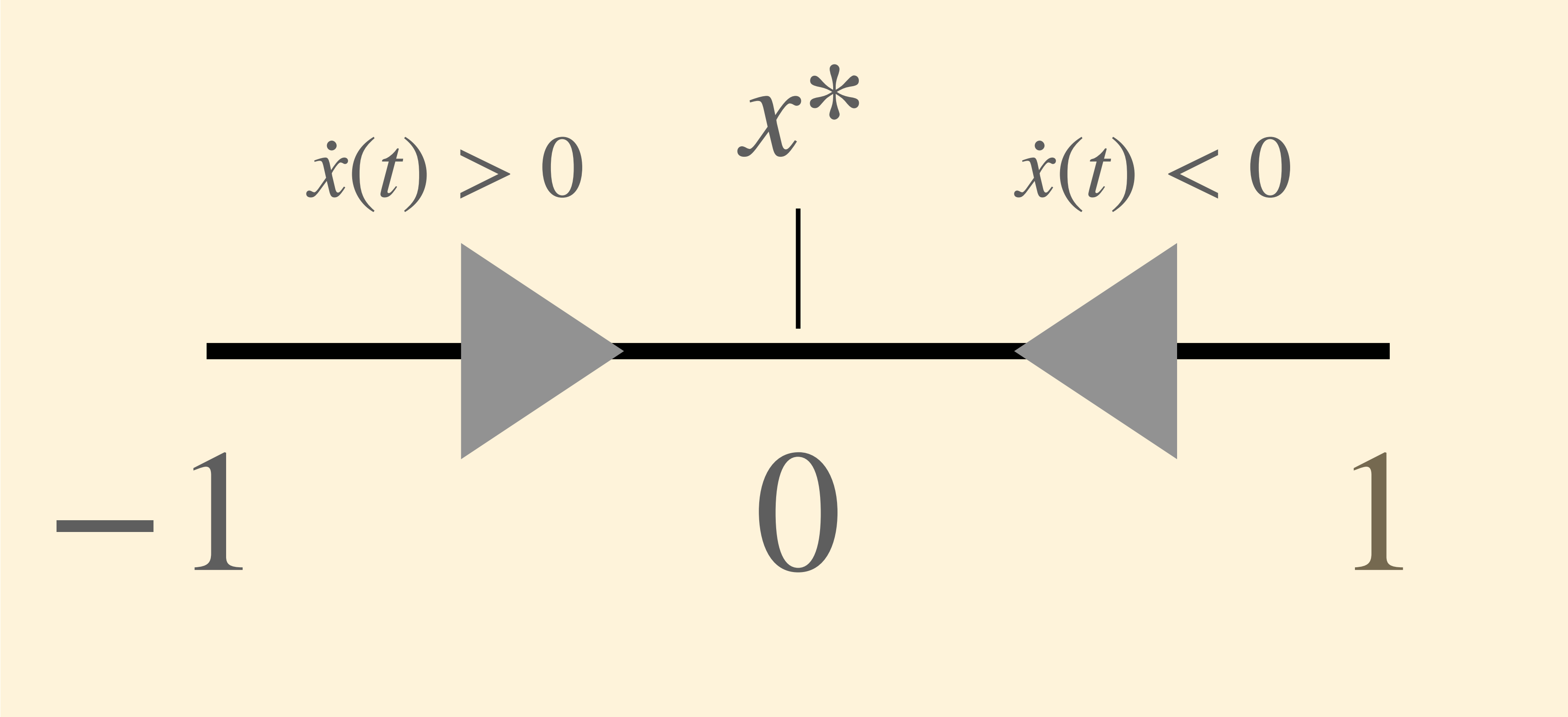
Fixed points for scalar ODE $\dot{x}(t) = f\big(x(t)\big)$

$$\dot{x}(t) = x(t)$$



$$\frac{\partial f}{\partial x} = 1 > 0$$

$$\dot{x}(t) = -x(t)$$



$$\frac{\partial f}{\partial x} = -1 < 0$$

Mathematical intuition $\dot{x}(t) = f(x(t), t)$

Fixed point:

$$f(x^*(t)) = 0$$

Small perturbation from fixed point:

$$x(t) = x^* + \delta x(t)$$

Taylor expansion of derivative:

(Finite difference approximation)

$$\overset{0}{\dot{x}^*} + \dot{\delta x}(t) \approx \overset{0}{f(x^*)} + \delta x(t) \frac{\partial f}{\partial x}(x^*)$$

Mathematical intuition

$$\dot{\delta x}(t) \approx \delta x(t) \frac{\partial f}{\partial x}(x^*)$$

$$\frac{\partial f}{\partial x} = 1 > 0 :$$

Perturbation grows (instability)

$$\frac{\partial f}{\partial x} = -1 < 0 :$$

Perturbation shrinks (stability)

Try for yourself

$$\dot{x}(t) = \sin\big(x(t)\big) - x(t)$$

$$\dot{x}(t) = x(t) - \sin\big(x(t)\big)$$

Fixed point at zero: For which of these ODEs is it stable/unstable?

Why was I so interested in the SIR model?

Most important skill in differential equation modelling is not maths

Practice at:

Making / justifying / criticising assumptions

Turning assumptions into equations

Turning equations into (qualified) insight

Further improvements?

Reinfection, superspreader events,
spatial modelling, …

Play with seminar code at home!