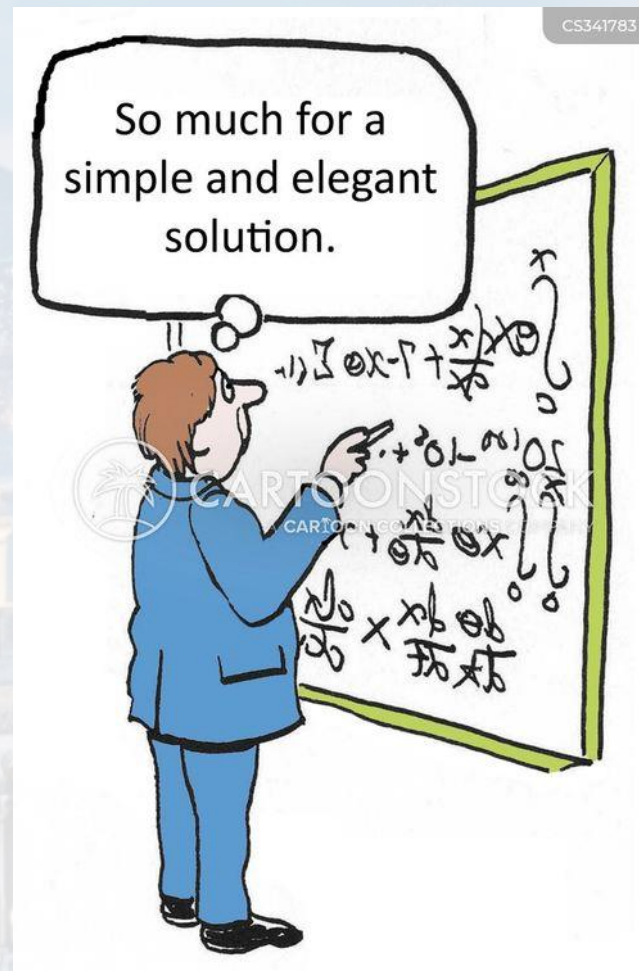


M. Hohle:

Physics 77: Introduction to Computational Techniques in Physics



syllabus:

- Introduction to Unix & Python (week 1 - 2)
- Functions, Loops, Lists and Arrays (week 3 - 4)
- Visualization (week 5)
- Parsing, Data Processing and File I/O (week 6)
- Statistics and Probability, Interpreting Measurements (week 7 - 8)
- Random Numbers, Simulation (week 9)
- Numerical Integration and Differentiation (week 10)
- Root Finding, Interpolation (week 11)
- Systems of Linear Equations (week 12)
- **Ordinary Differential Equations (week 13)**
- Fourier Transformation and Signal Processing (week 14)
- Capstone Project Presentations (week 15)



ordinary differential equation:

- **total** derivative \rightarrow *ordinary*

$$\frac{d^k f(x)}{dx^k} \quad k \in \mathbb{N}$$

- of **n-th** order $\rightarrow n = \max(k)$

- **non-linear** \rightarrow *power of **any** x is not one*

partial differential equation:

- at least one **partial** derivative

$$\frac{\partial y(x)}{\partial t} = [a\Delta + bg(x)] y(x)$$

diffusion

$$\frac{\partial^2 y(x)}{\partial t^2} = [a\Delta + bg(x)] y(x)$$

wave

What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python



let's start simple:

constant **relative change** per **time step**

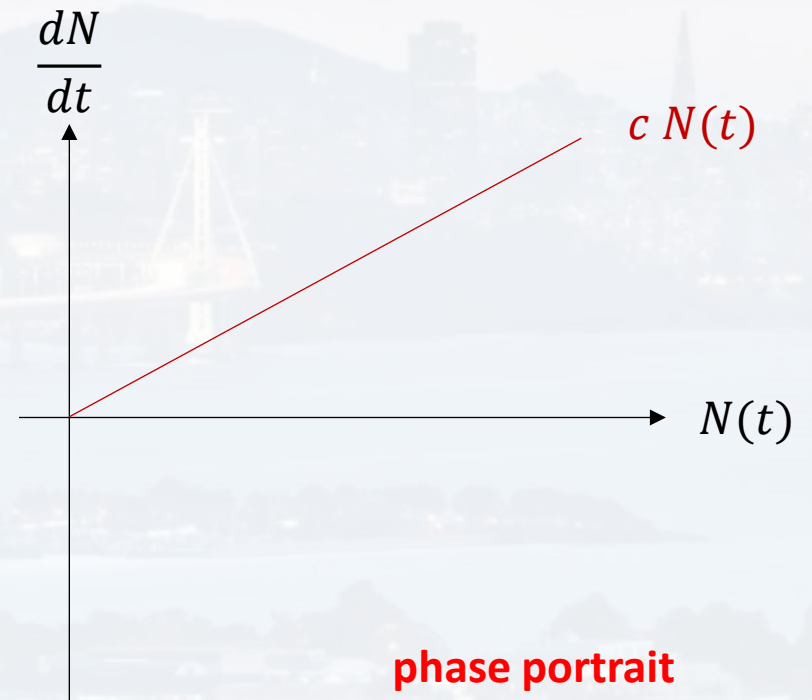
$$\frac{\Delta N}{N} \frac{1}{\Delta t} = c$$

$$\frac{dN}{N} = c dt$$

$$\frac{dN}{dt} = c N$$

$$\int_{N(t=0)}^N \frac{1}{N} dN = c \int_0^\tau dt$$

$$N(t) = N(t=0) e^{ct}$$



What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python



let's start simple:

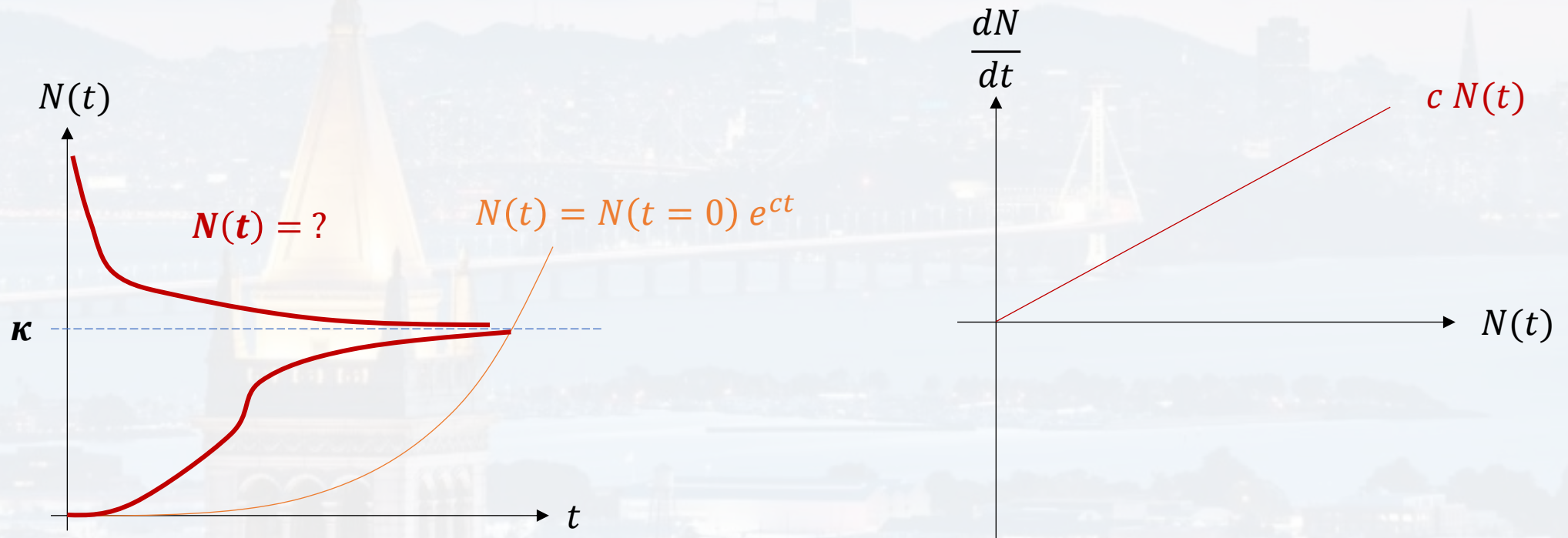
What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python

We want the model to have a limited carrying capacity κ

$$\frac{dN}{N} = c dt$$





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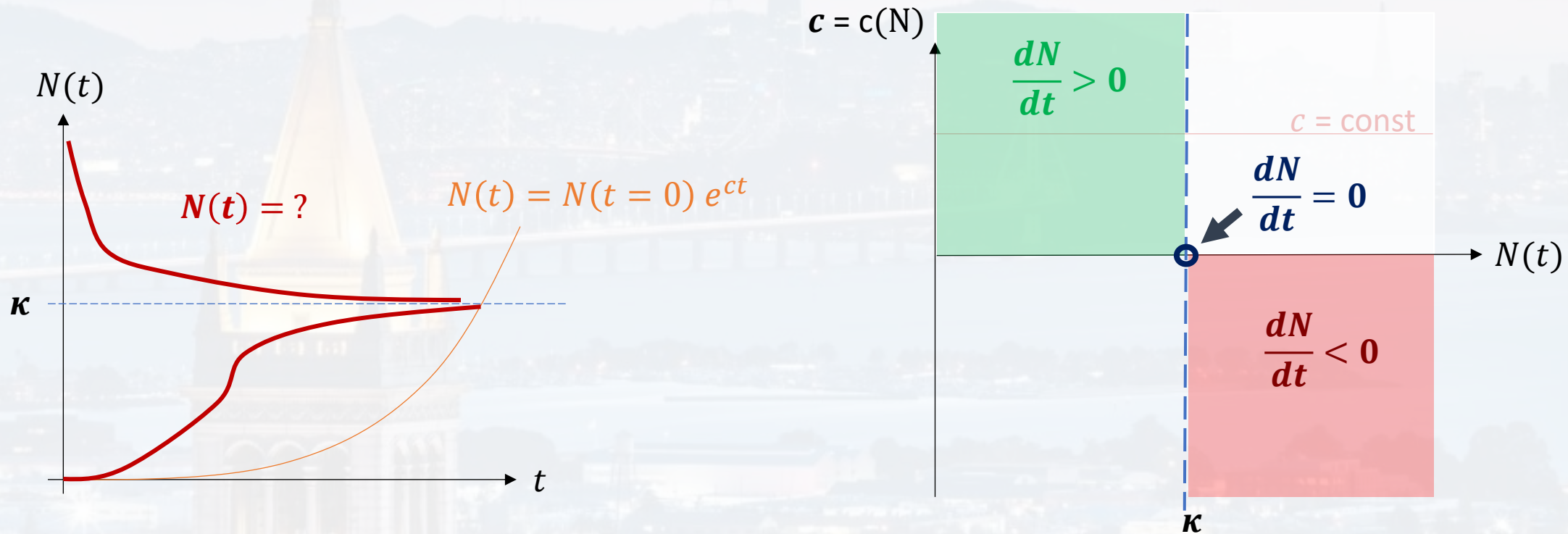
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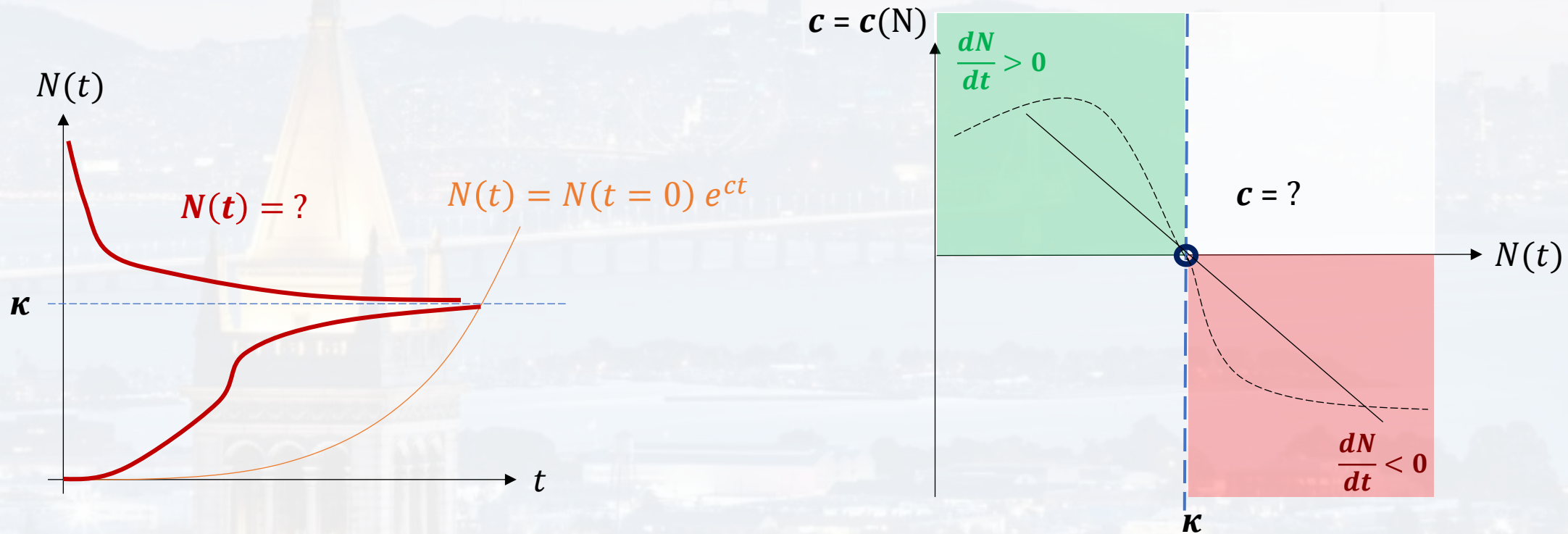
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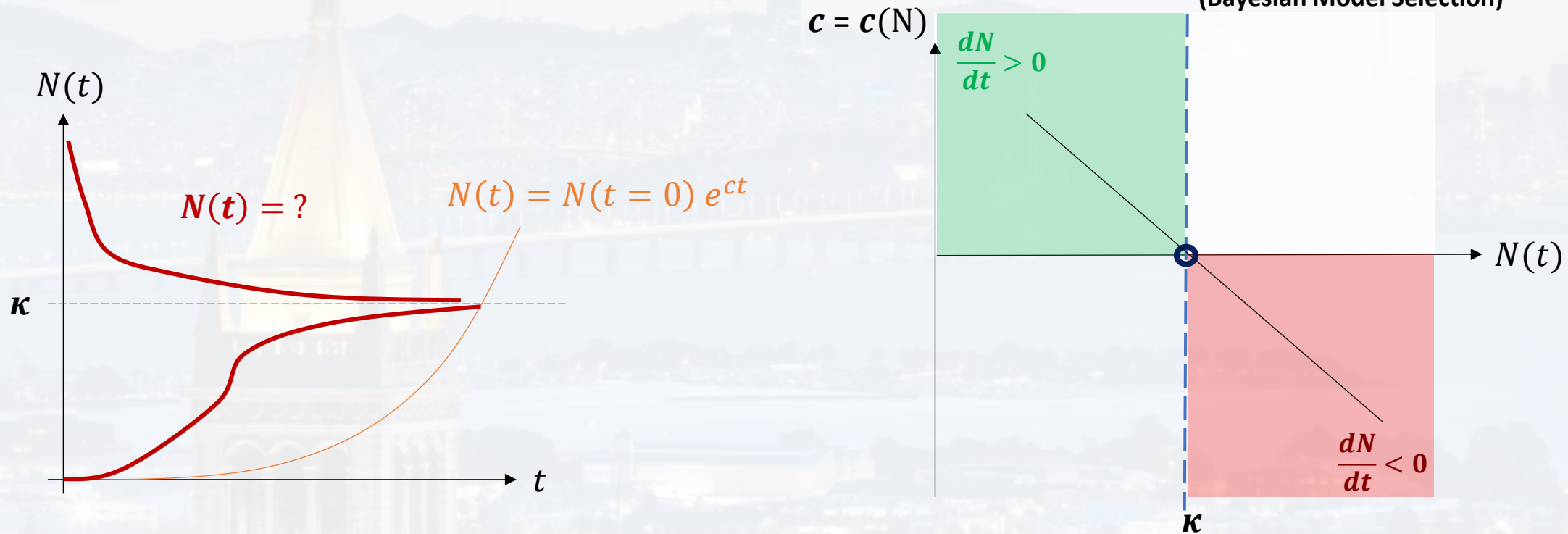
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Solving ODEs by thinking

Solving ODEs with Python

Occam's razor:

prefer simple model
(Bayesian Model Selection)





let's start simple:

We want the model to have a limited carrying capacity κ

$$\frac{dN}{N} = c dt$$

$$c(N) = c_0 + m N$$

$$c(\kappa) = 0 \quad c(\kappa) = 0 = c_0 + m \kappa \quad m = -\frac{c_0}{\kappa}$$

$$c(0) = c_0$$

$$c(N) = c_0 \left(1 - \frac{1}{\kappa} N \right)$$

$$\frac{dN}{N} = c_0 \left(1 - \frac{1}{\kappa} N \right) dt$$

Verhulst Equation

$c = c(N)$

$\frac{dN}{dt} > 0$

κ

$\frac{dN}{dt} < 0$

$N(t)$

What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python

Occam's razor:

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(Bayesian Model Selection)



let's start simple:

What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python

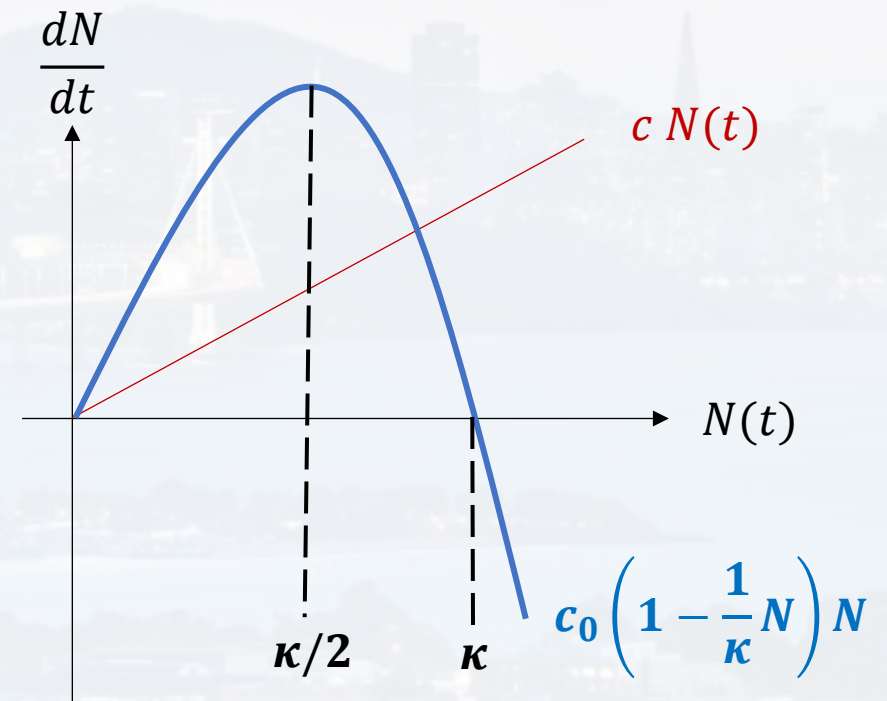
We want the model to have a limited carrying capacity κ

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Verhulst Equation

$$\frac{dN}{dt} = c_0 \left(1 - \frac{1}{\kappa} N \right) N$$





let's start simple:

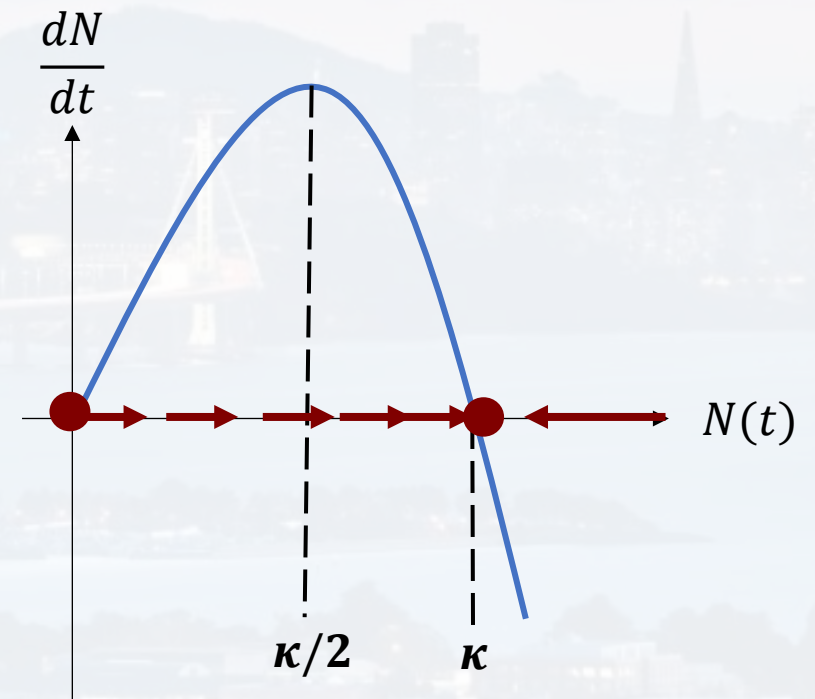
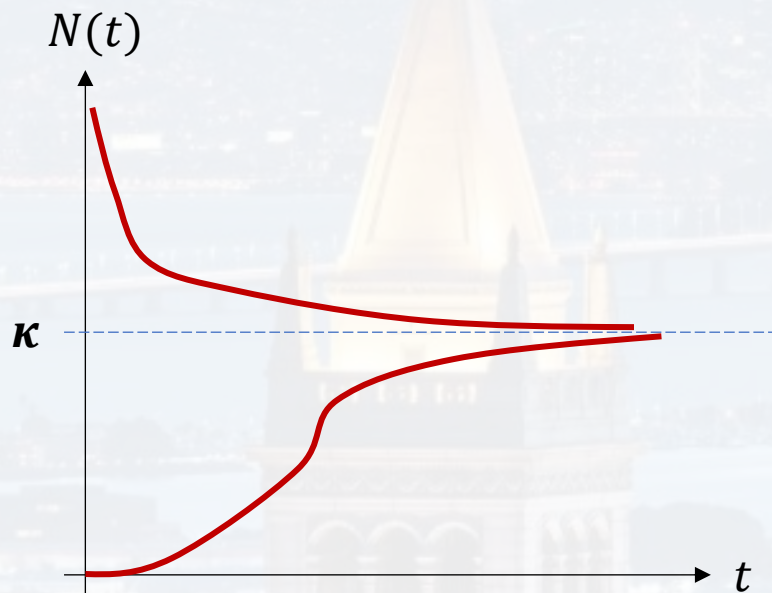
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Solving ODEs by thinking

Solving ODEs with Python

We want the model to have a limited carrying capacity κ

$$\frac{dN}{dt} = c_0 \left(1 - \frac{1}{\kappa} N \right) N \quad \text{Verhulst Equation}$$





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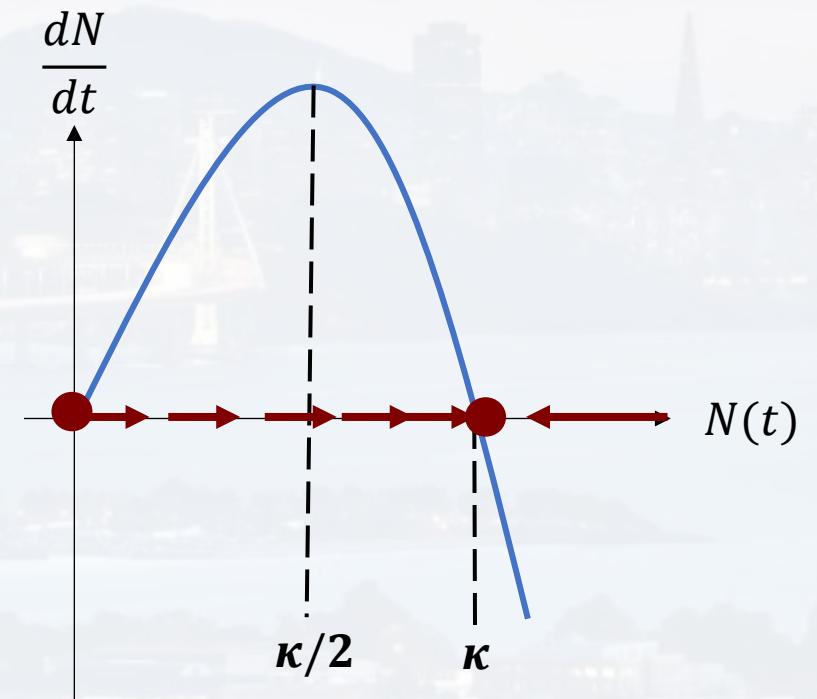
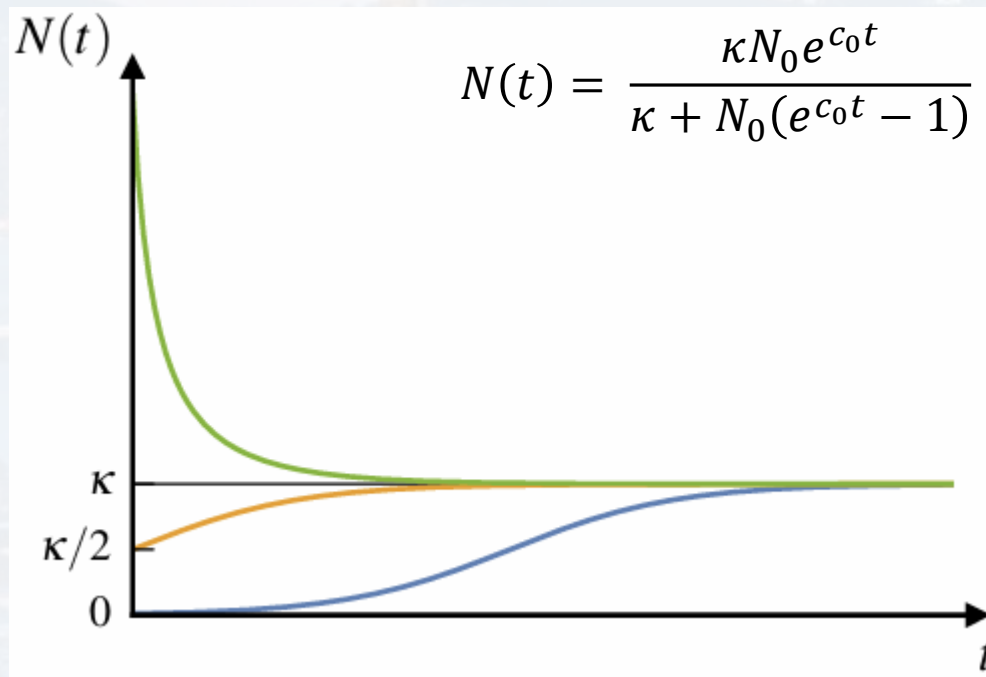
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Solving ODEs by thinking

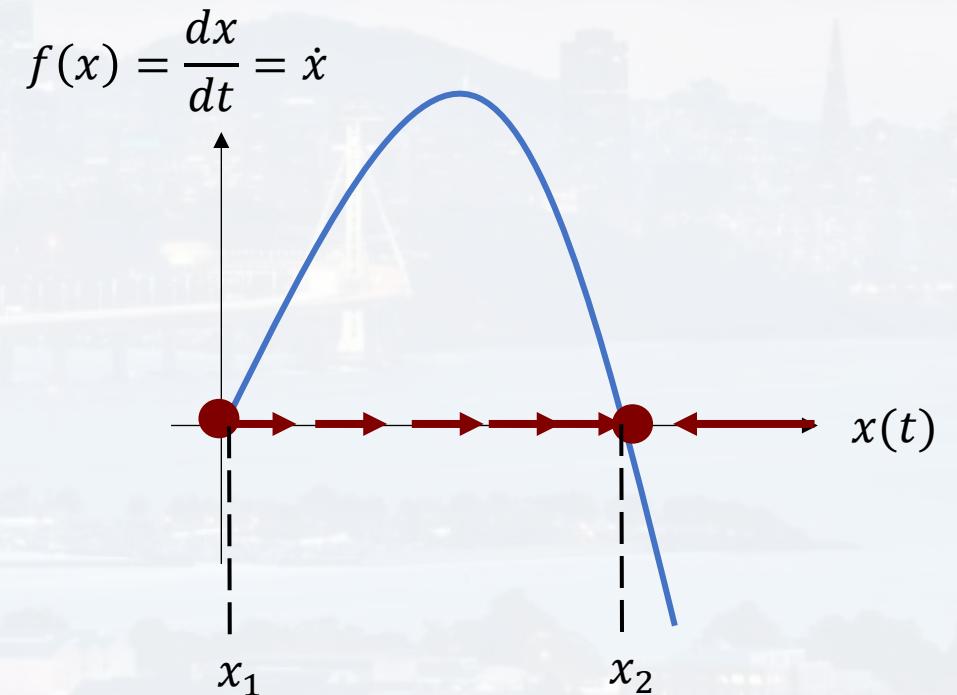
Solving ODEs with Python

We want the model to have a limited carrying capacity κ

$$\frac{dN}{dt} = c_0 \left(1 - \frac{1}{\kappa} N \right) N \quad \text{Verhulst Equation}$$

x_1, x_2 fixed points

$$f(x) = \frac{dx}{dt} = \dot{x}$$





fixed points x^*

x_1 : repeller

→ unstable

$$\frac{df(x)}{dx} = \frac{d}{dx}\dot{x} > 0$$

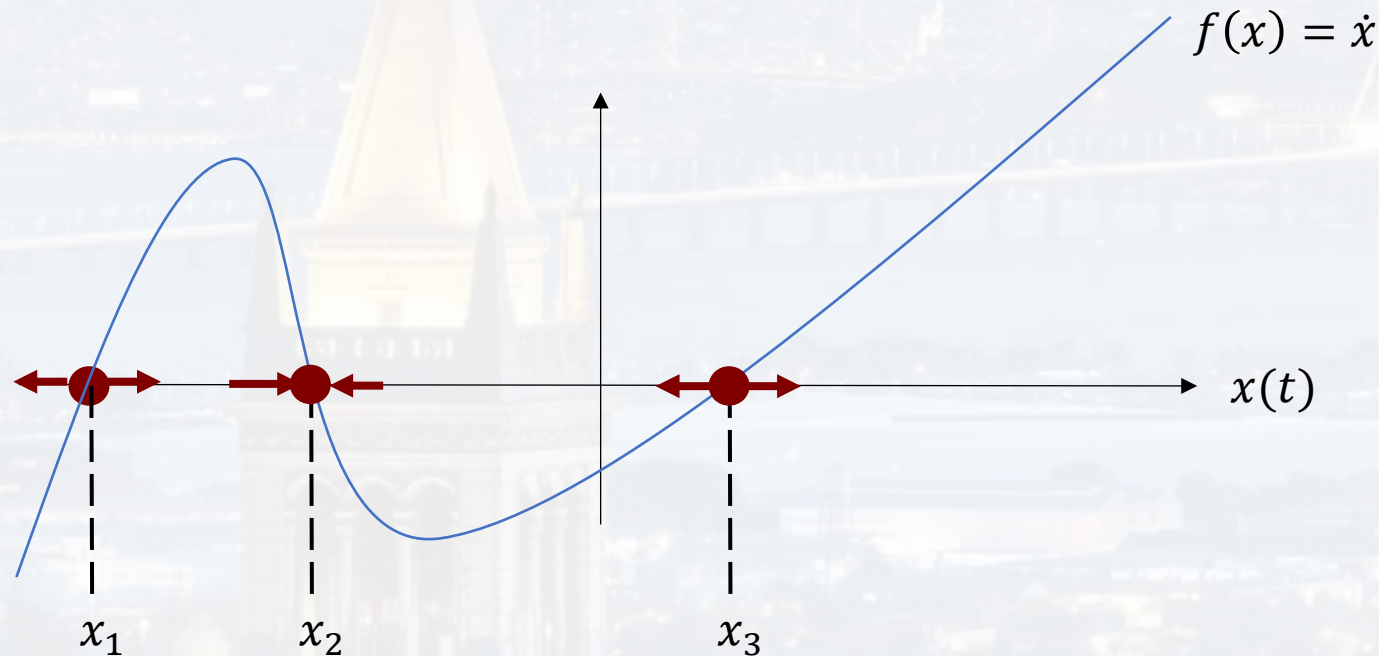
x_3 : repeller

→ unstable

x_2 : attractor

→ stable

$$\frac{df(x)}{dx} = \frac{d}{dx}\dot{x} < 0$$



What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python



fixed points x^*

small perturbation $\varepsilon(t)$

What is an ODE?

Solving ODEs by thinking

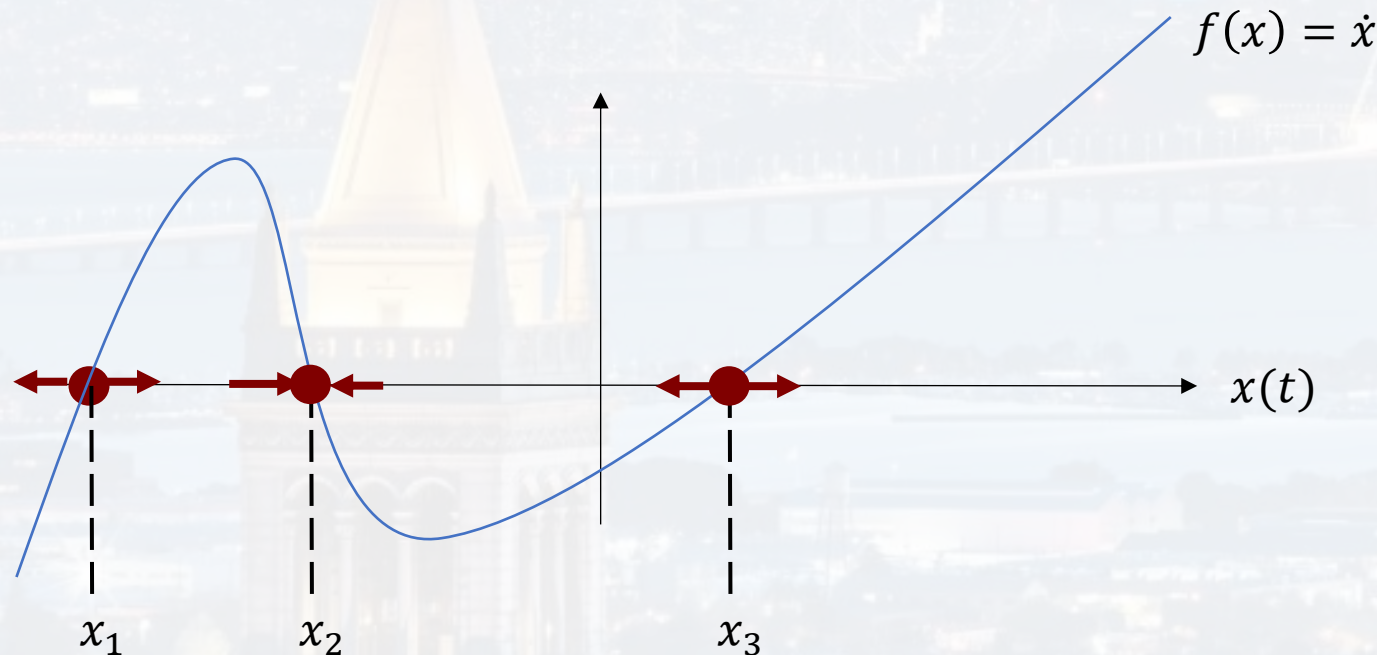
Solving ODEs with Python

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

$$\frac{d\varepsilon(t)}{dt} = \frac{d}{dt}[x(t) - x^*] = f(x) + 0 = f(x^* + \varepsilon(t))$$

$$\boxed{\frac{d\varepsilon(t)}{dt}} = f(x^* + \varepsilon(t)) \approx f(x^*) + \left. \frac{df(x)}{dx} \right|_{x=x^*} \varepsilon(t) = 0 + \boxed{\left. \frac{df(x)}{dx} \right|_{x=x^*} \varepsilon(t)}$$

$$\boxed{\varepsilon(t) = \varepsilon_0 e^{\left. \frac{df(x)}{dx} \right|_{x=x^*} t}}$$



$$\text{time scale } \tau = \frac{1}{\left. \frac{df(x)}{dx} \right|_{x=x^*}}$$

$$\frac{df(x)}{dx} > 0 \quad \text{unstable}$$

$$\frac{df(x)}{dx} < 0 \quad \text{stable}$$



fixed points x^*

small perturbation $\varepsilon(t)$

What is an ODE?

Solving ODEs by thinking

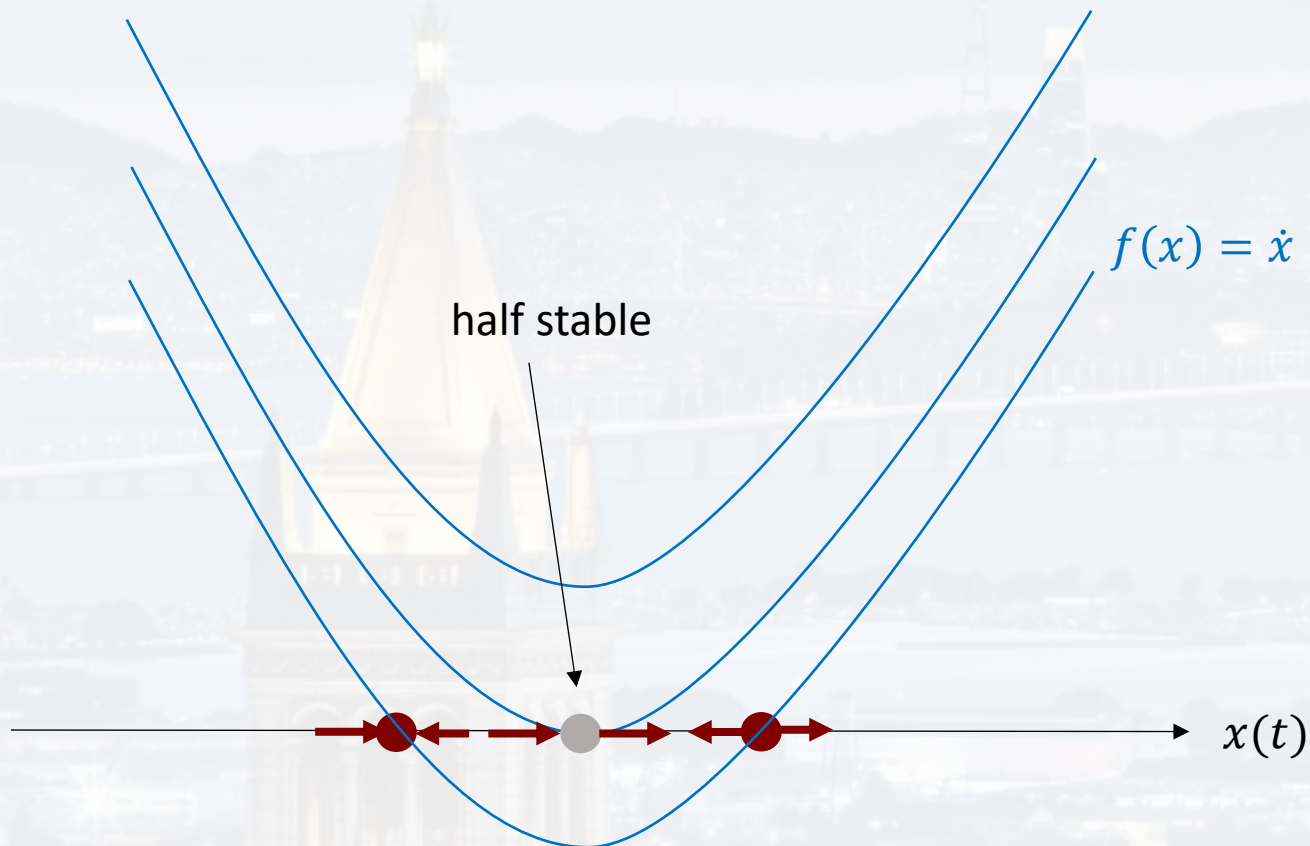
Solving ODEs with Python

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What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python

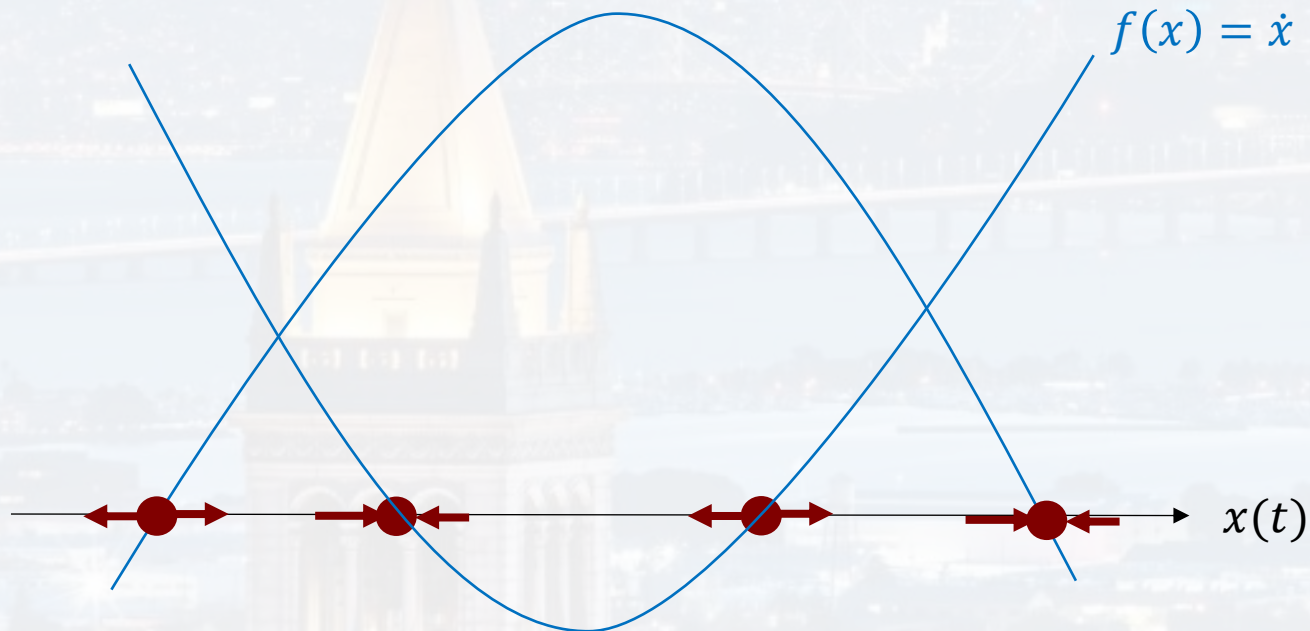
$$\varepsilon(t) = \varepsilon_0 e^{\frac{df(x)}{dx}|_{x=x^*} t}$$

$$\text{time scale } \tau = \frac{1}{\frac{df(x)}{dx}|_{x=x^*}}$$

$$f(x) = ax^2 + bx + c$$

$$\frac{df(x)}{dx} > 0 \quad \text{unstable}$$

$$\frac{df(x)}{dx} < 0 \quad \text{stable}$$



if coupled to another system: \rightarrow can change dynamics drastically (chem reactions)



2D system

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

$$\dot{x} = -x + a y + x^2 y$$

$$g(x, y) = \dot{y}$$

$$\dot{y} = b - a y - x^2 y$$

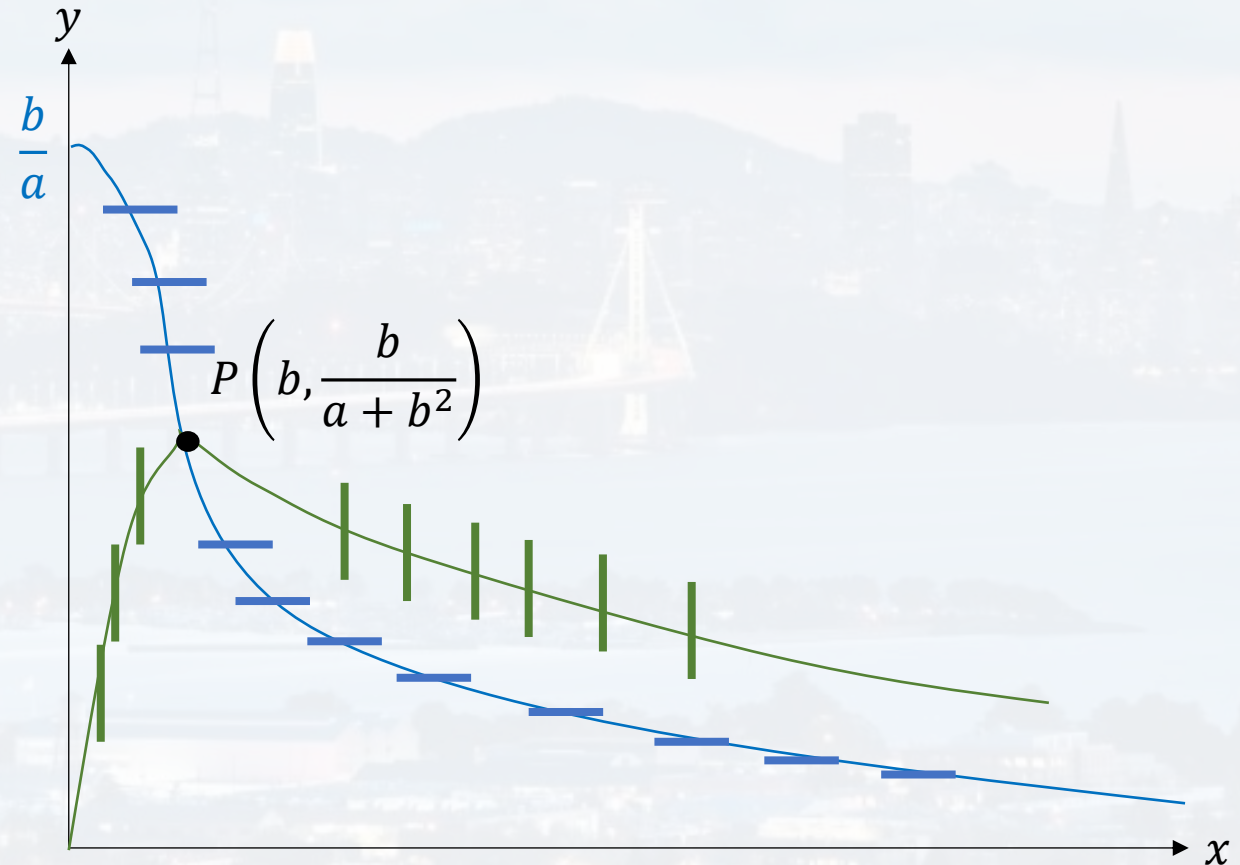
non-linear, coupled ODEs

null clines

$$\dot{x} = 0 \rightarrow y_1 = \frac{x}{a + x^2}$$

$$\dot{y} = 0 \rightarrow y_2 = \frac{b}{a + x^2}$$

Find out which way the system moves!



What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python



2D system

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$$\dot{x} = -x + a y + x^2 y$$

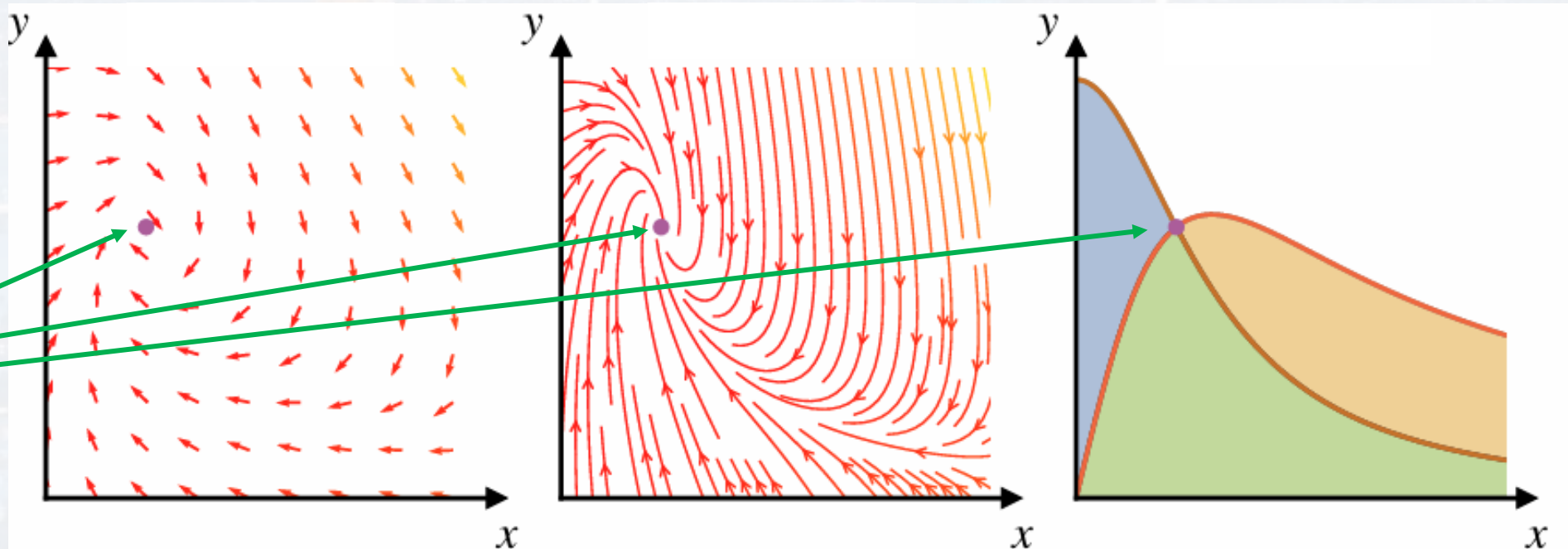
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non-linear, coupled ODEs

$$\dot{x} = 0 \Rightarrow y_1 = \frac{x}{a + x^2}$$

$$\dot{y} = 0 \Rightarrow y_2 = \frac{b}{a + x^2}$$



attractor or
repeller?

What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python



2D system

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

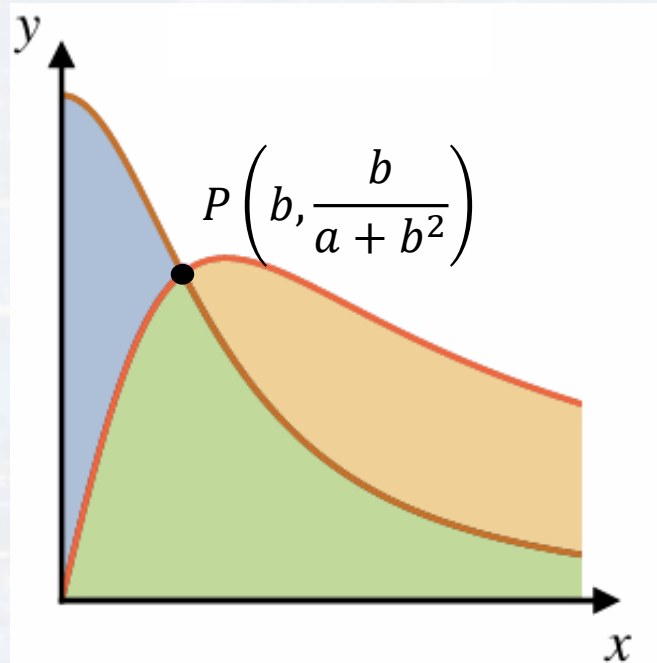
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non-linear, coupled ODEs

stability of P:



$$\frac{d \varepsilon_x(t)}{dt} \approx f(x^* + \varepsilon_x, y^* + \varepsilon_y) \approx f(x^*, y^*) + \underbrace{\frac{\partial f(x, y)}{\partial x} \Big|_{x^*, y^*}}_a \varepsilon_x + \underbrace{\frac{\partial f(x, y)}{\partial y} \Big|_{x^*, y^*}}_b \varepsilon_y$$

$$\frac{d \varepsilon_y(t)}{dt} \approx g(x^* + \varepsilon_x, y^* + \varepsilon_y) \approx g(x^*, y^*) + \underbrace{\frac{\partial g(x, y)}{\partial x} \Big|_{x^*, y^*}}_c \varepsilon_x + \underbrace{\frac{\partial g(x, y)}{\partial y} \Big|_{x^*, y^*}}_d \varepsilon_y$$

$= 0$

$$\dot{\vec{\varepsilon}} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \vec{\varepsilon}$$

What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python



2D system

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

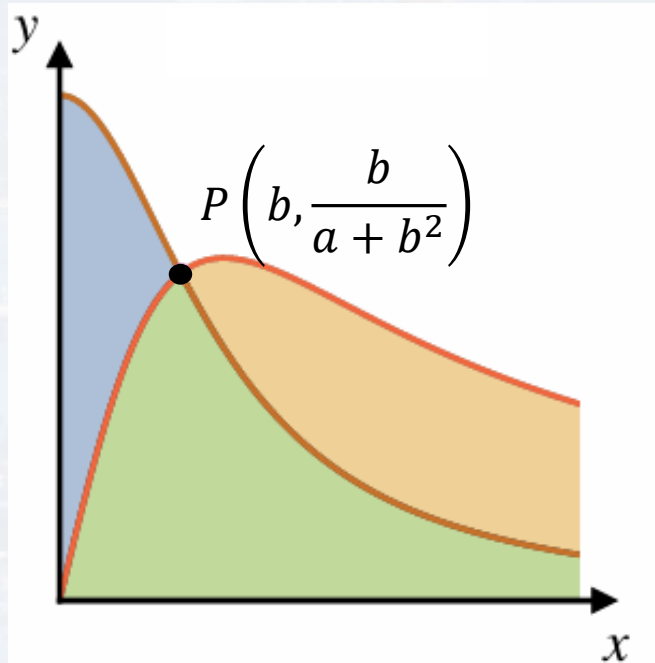
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non-linear, coupled ODEs

stability of P:



$$\dot{\vec{\epsilon}} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \vec{\epsilon} \quad A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

$$\epsilon(t) = \epsilon_0 e^{\frac{df(x)}{dx}|_{x=x^*} t}$$

$$\vec{\epsilon}(t) = \vec{\epsilon}(t=0) e^{\lambda t}$$

λ : eigenvalue of A

What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python



2D system

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

$$\dot{x} = -x + a y + x^2 y$$

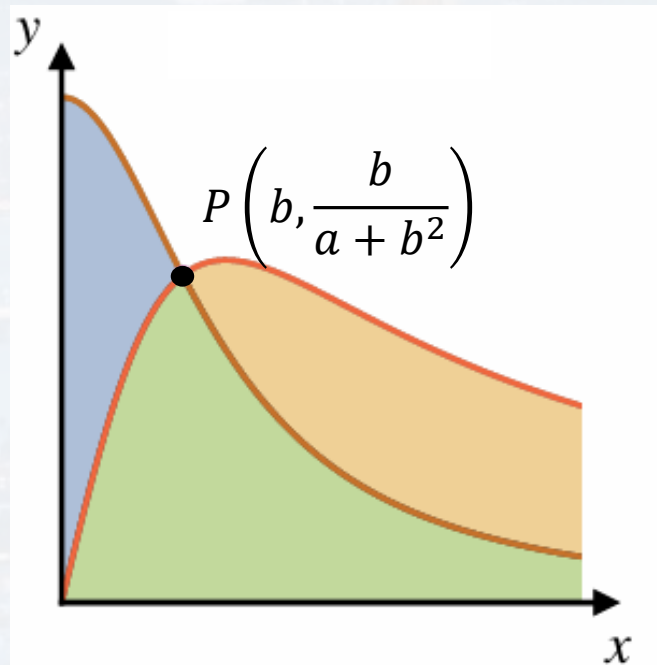
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non-linear, coupled ODEs

stability of P:

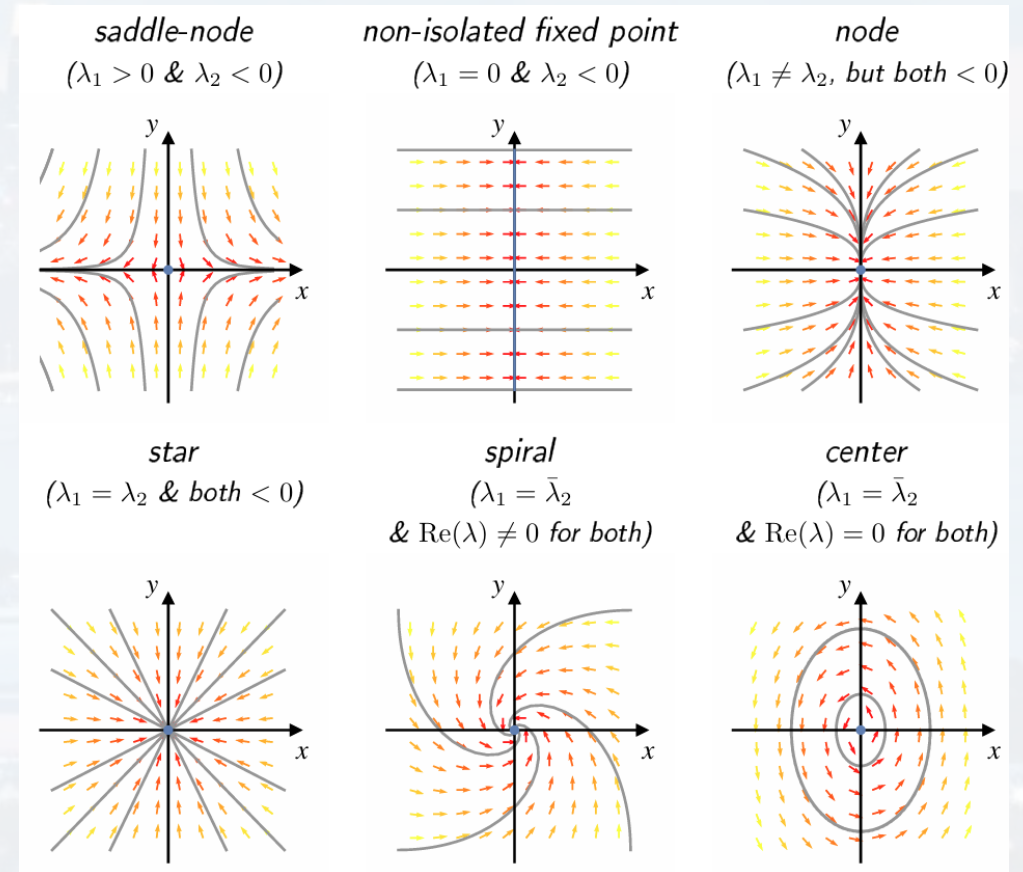
$$\vec{\epsilon}(t) = \vec{\epsilon}(t=0) e^{\lambda t}$$



What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python





2D system

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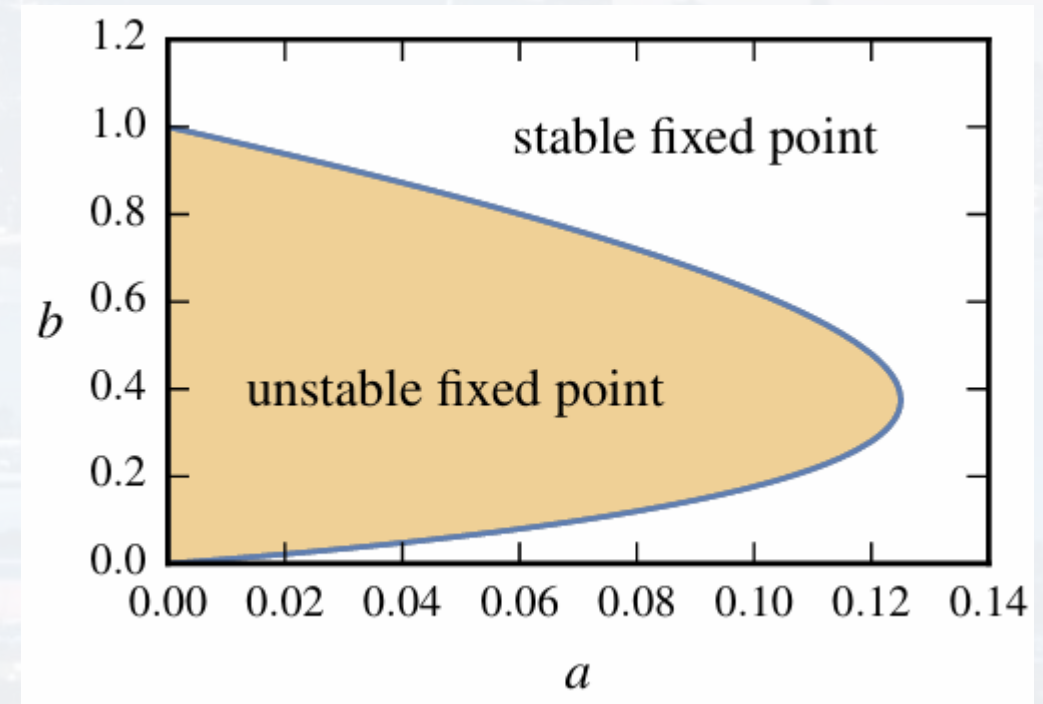
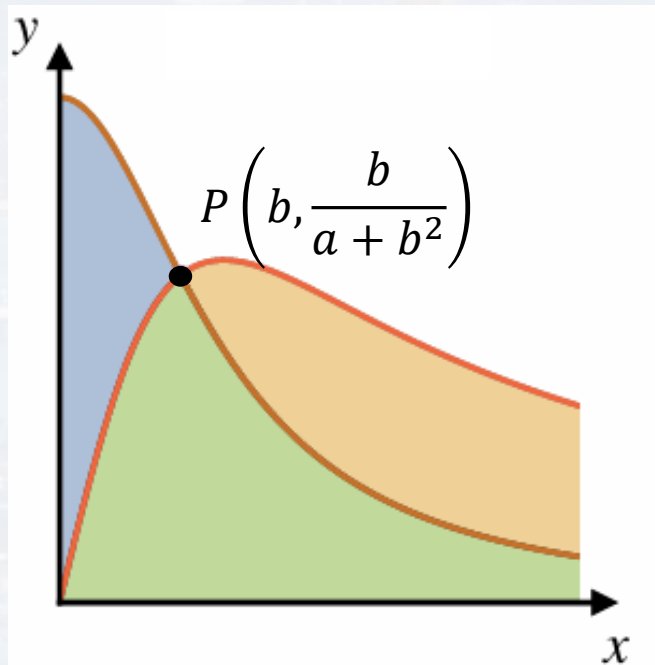
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non-linear, coupled ODEs

stability of P:

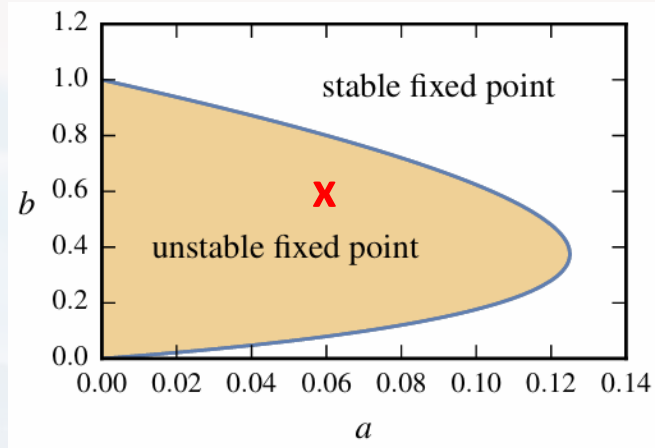
$$\vec{\epsilon}(t) = \vec{\epsilon}(t=0) e^{\lambda t}$$

for this particular system:

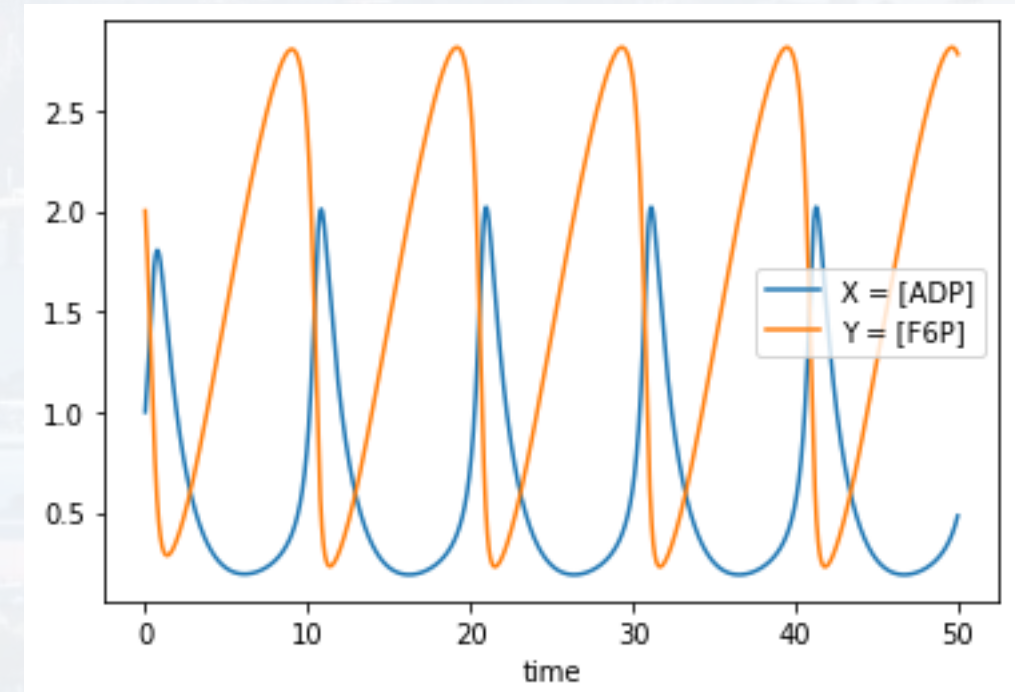
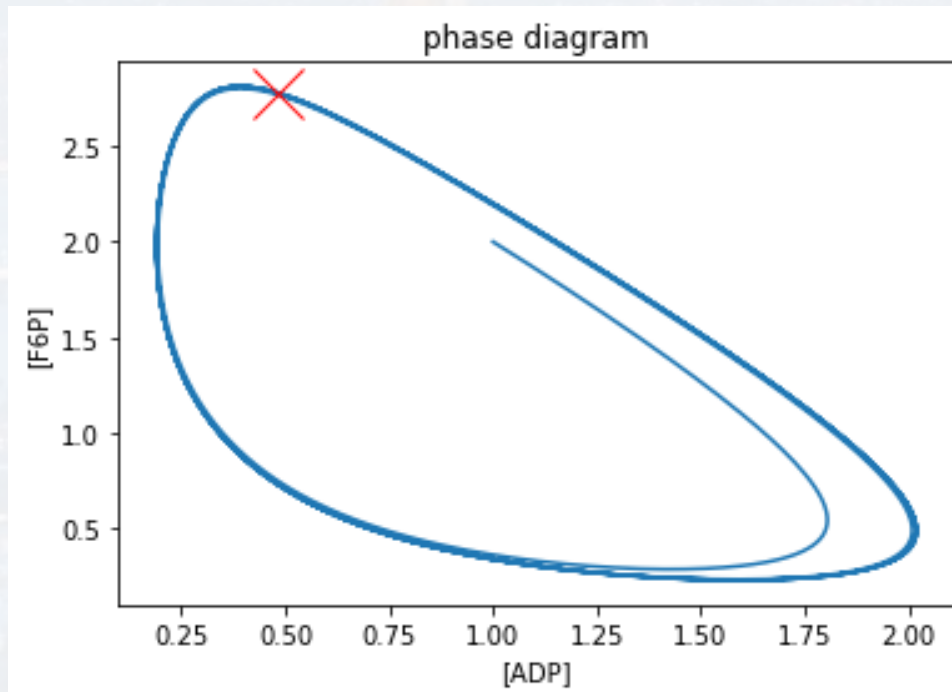




2D system



$$P\left(b, \frac{b}{a + b^2}\right) = (0.6, 1.42)$$



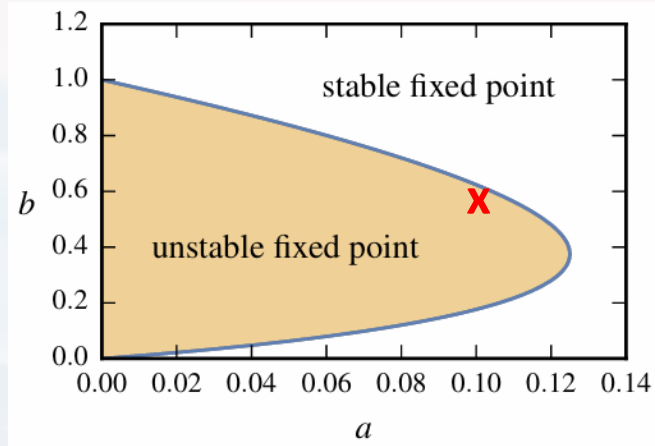
What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python



2D system

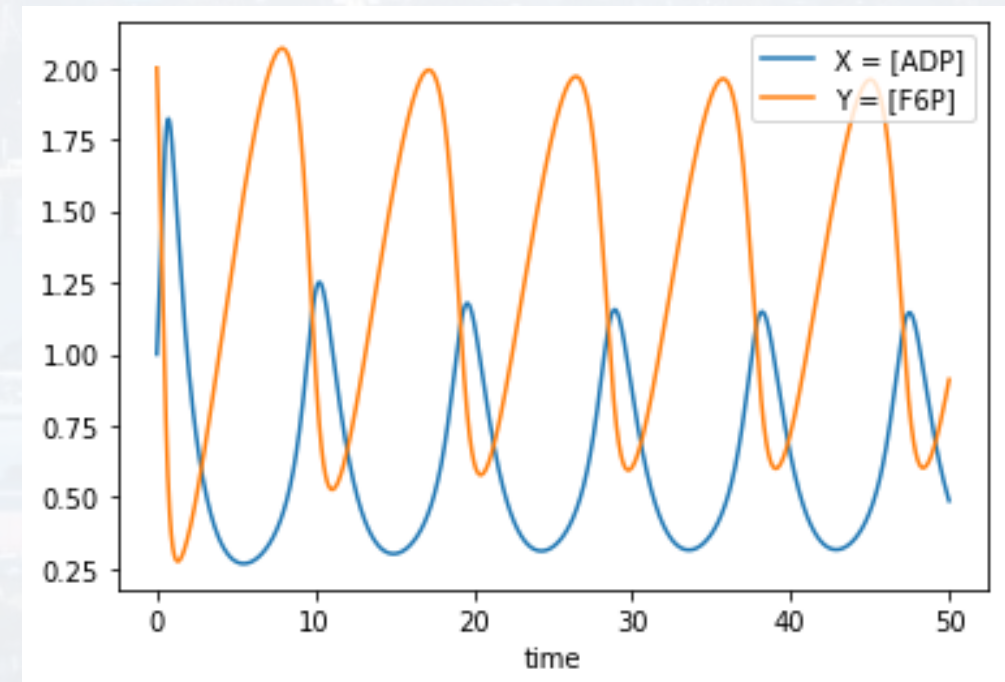
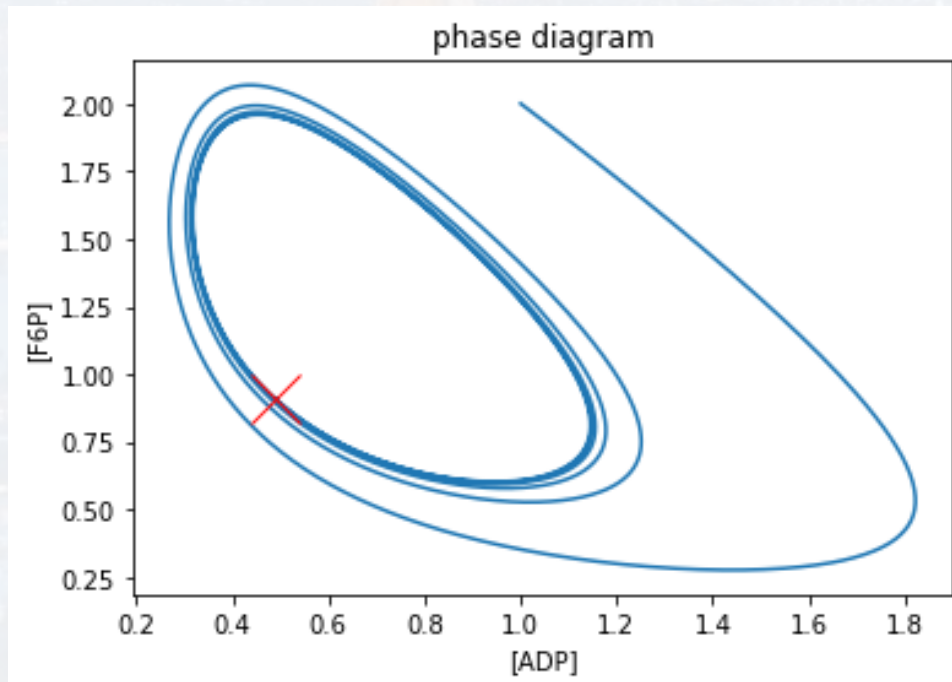


$$P\left(b, \frac{b}{a + b^2}\right) = (0.6, 1.30)$$

What is an ODE?

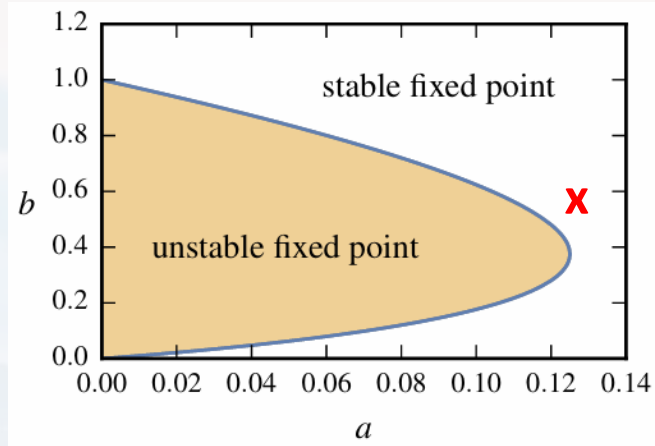
Solving ODEs by thinking

Solving ODEs with Python





2D system

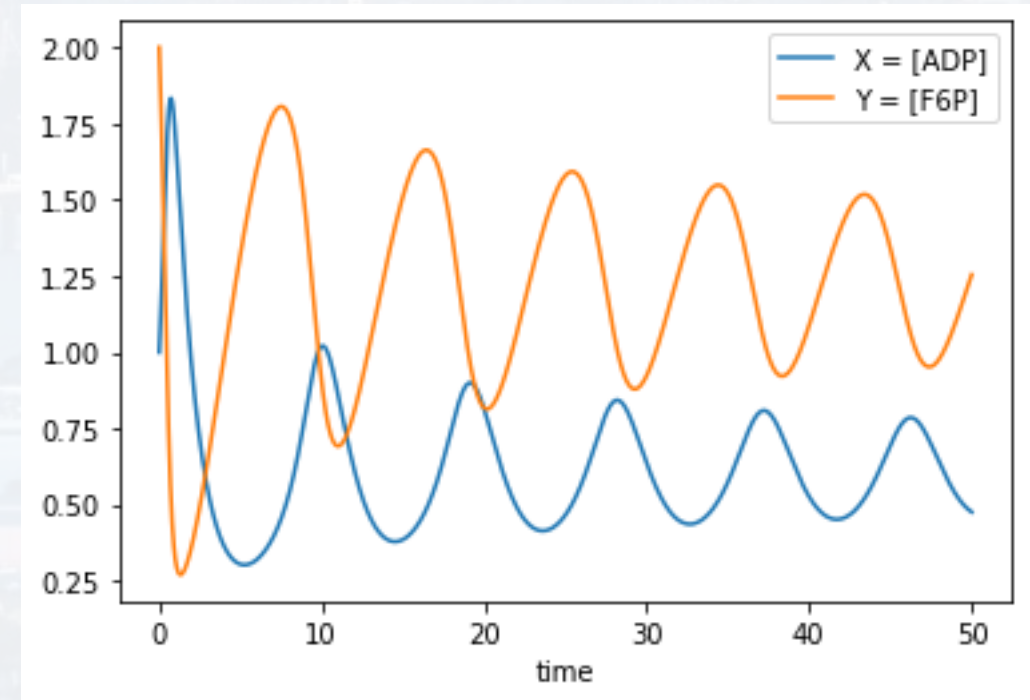
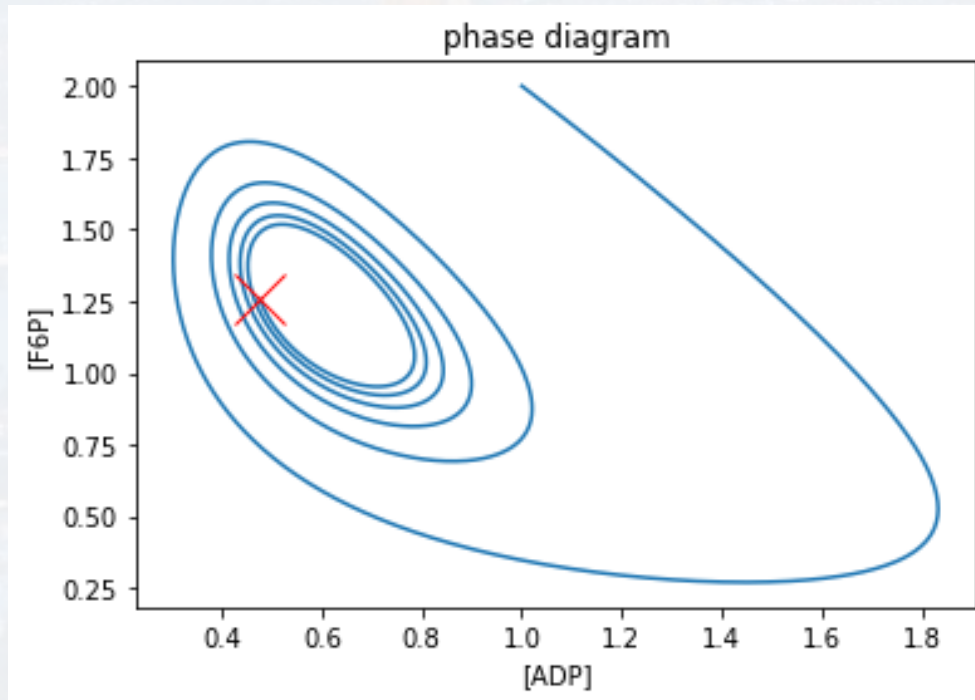


$$P\left(b, \frac{b}{a + b^2}\right) = (0.6, 1.24)$$

What is an ODE?

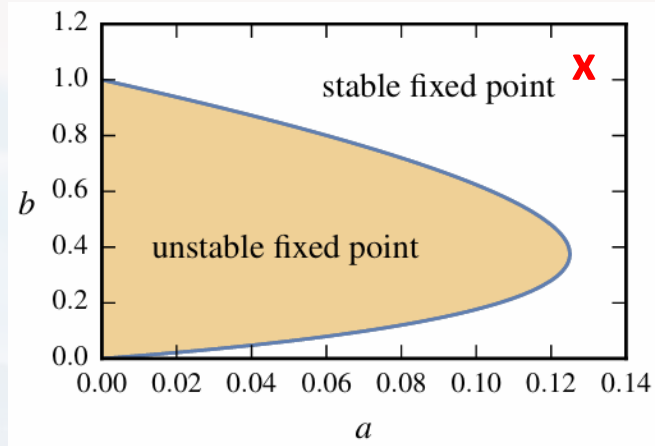
Solving ODEs by thinking

Solving ODEs with Python





2D system

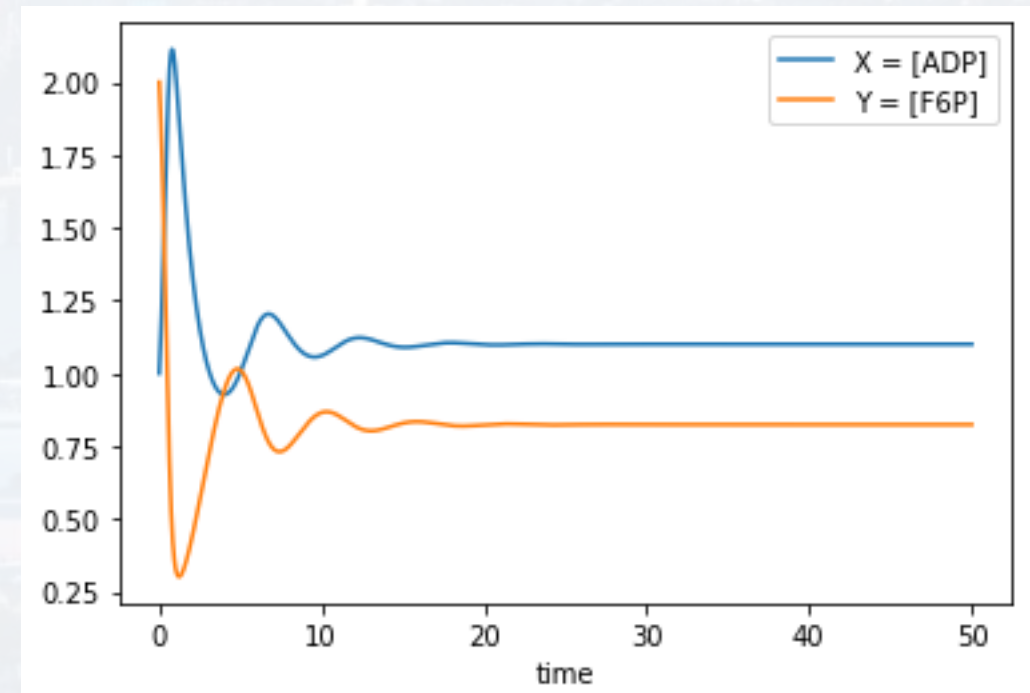
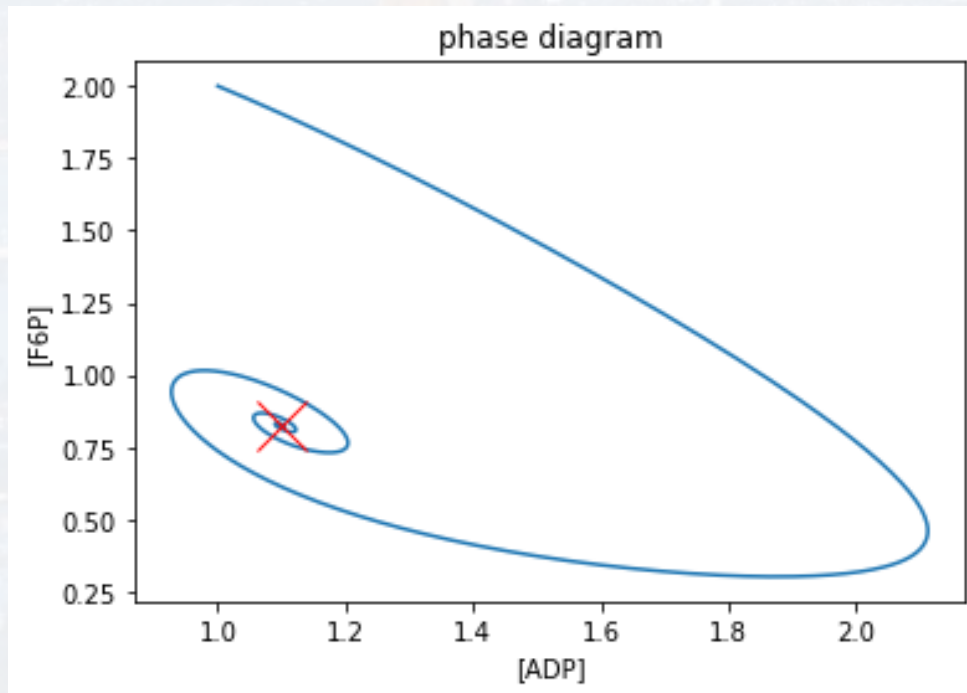


$$P\left(b, \frac{b}{a + b^2}\right) = (1.1, 0.82)$$

What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python





Runge-Kutta-Heun

What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python

$$\frac{dy}{dt} = f(x(t), t)$$

initial condition: $y_0 = y(t_0)$

goal: $y(t)$

$$y(t + dt) = y(t) + \frac{dy}{dt} dt + \frac{1}{2} \frac{d^2 y}{dt^2} dt^2 + \dots$$

$$y(t + dt) = y(t) + f(x, t) dt + \frac{1}{2} \frac{d}{dt} f(x, t) dt^2 + \dots$$

$$y(t + dt) = y(t) + f(x, t) dt + \frac{1}{2} \left[\frac{\partial f}{\partial x} \frac{dx}{dt} + \frac{\partial f}{\partial t} \right] dt^2 + \dots$$

note: more general $\frac{dy}{dx} = f(x(t), y(x(t)))$



Runge-Kutta-Heun

```
from scipy.integrate import solve_ivp
```

```
method = 'RK45'
```

4: referring to the number of subintervals for integration (4 is equivalent to the Simpson rule)

5: referring to the order of the Taylor approximation for the derivatives

What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python



$$\dot{x} = -x + a y + x^2 y$$

$$\dot{y} = b - a y - x^2 y$$

What is an ODE?
Solving ODEs by thinking
Solving ODEs with Python

```
def SolveGlycolysis(Init, t_span, a, b):
    XY = ode_solver(Glycolysis, Init, t_span, method = 'RK45',\
                     a = a, b = b)

    t = XY.t
    X = XY.y[0,:]
    Y = XY.y[1,:]

    #####plotting result#####

    #...
```



$$\dot{x} = -x + a y + x^2 y$$

$$\dot{y} = b - a y - x^2 y$$

What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python

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```

```
    XY = ode_solver(Glycolysis, Init, t_span, method = 'RK45',\n                    a = a, b = b)
```

```
def Glycolysis(Init, t, a, b):
```

```
    x = Init[0]
```

```
    y = Init[1]
```

```
    dx = -x + a*y + (x**2)*y
```

```
    dy = b - a*y - (x**2)*y
```

```
    D = [dx, dy]
```

```
    return D
```

note: t is an input
variable, even though it is
not being used explicitly
→ integration over t



$$\dot{x} = -x + a y + x^2 y$$

$$\dot{y} = b - a y - x^2 y$$

What is an ODE?

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Solving ODEs with Python

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```
    t = XY.t
    X = XY.y[0,:]
    Y = XY.y[1,:]
```

```
#####plotting result#####
```

```
#...
```

the actual solver



$$\dot{x} = -x + a y + x^2 y$$

$$\dot{y} = b - a y - x^2 y$$

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    XY = ode_solver(Glycolysis, Init, t_span, method = 'RK45',\n                    a = a, b = b)
```

```
from scipy.integrate import solve_ivp
```

```
def ode_solver(ode_func, Init, t_span, method = 'RK45', **params):
```

```
    result = solve_ivp(fun = lambda t, y: ode_func(y, t, **params),\n                       t_span = t_span, y0 = Init, method = method,\n                       rtol = 1e-9, atol = 1e-9, max_step = 0.01)
```

```
    return result
```



$$\dot{x} = -x + a y + x^2 y$$

$$\dot{y} = b - a y - x^2 y$$

What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python

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```

```
    result = solve_ivp(fun = lambda t, y: ode_func(y, t, **params),\n                      t_span = t_span, y0 = Init, method = method,\n                      rtol = 1e-9, atol = 1e-9, max_step = 0.01)
```

```
    return result
```



$$\dot{x} = -x + a y + x^2 y$$

$$\dot{y} = b - a y - x^2 y$$

run:

$a = 0.125$

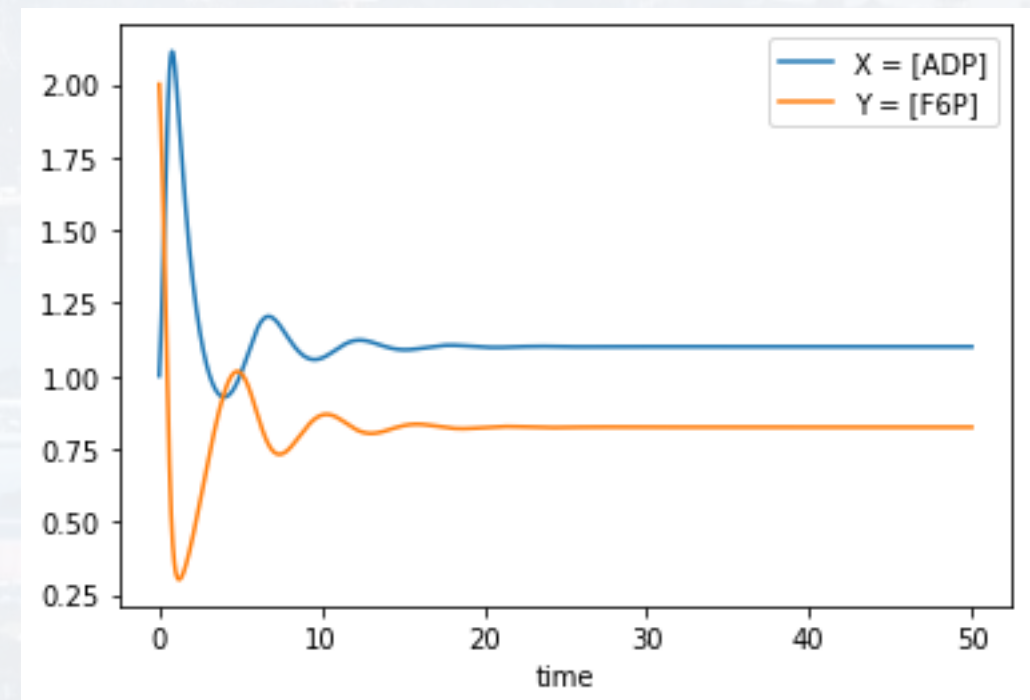
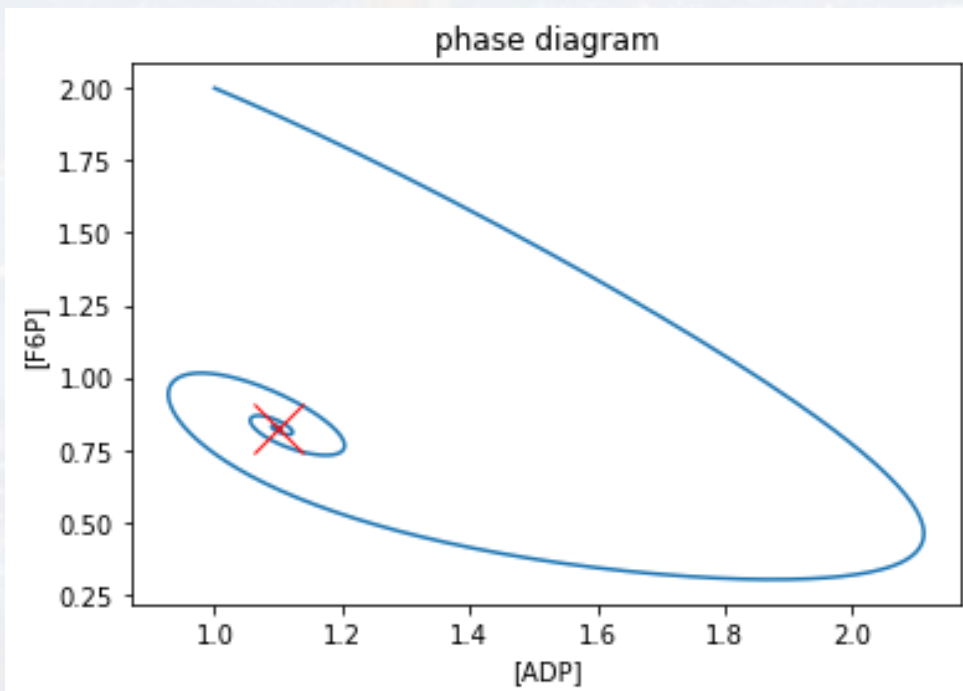
$b = 1.1$

`SolveGlycolysis([1, 2], [0, 50], a, b)`

What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python





run:

SolvePhageTherapy(Init, t_span, rates)

Synergistic elimination of bacteria by phage and the immune system

Chung Yin (Joey) Leung* and Joshua S. Weitz†
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$$\begin{aligned}\dot{B} &= \overbrace{rB(1 - \frac{B}{K_C})}^{\text{Growth}} - \overbrace{\phi BP}^{\text{Lysis}} - \overbrace{\frac{\epsilon IB}{1 + B/K_D}}^{\text{Immune killing}}, \\ \dot{P} &= \overbrace{\beta \phi BP}^{\text{Replication}} - \overbrace{\omega P}^{\text{Decay}}, \\ \dot{I} &= \overbrace{\alpha I(1 - \frac{I}{K_I}) \frac{B}{B + K_N}}^{\text{Immune stimulation}}.\end{aligned}$$

B: bacteria
P: phages
I: immune cells

What is an ODE?

Solving ODEs by thinking

Solving ODEs with Python

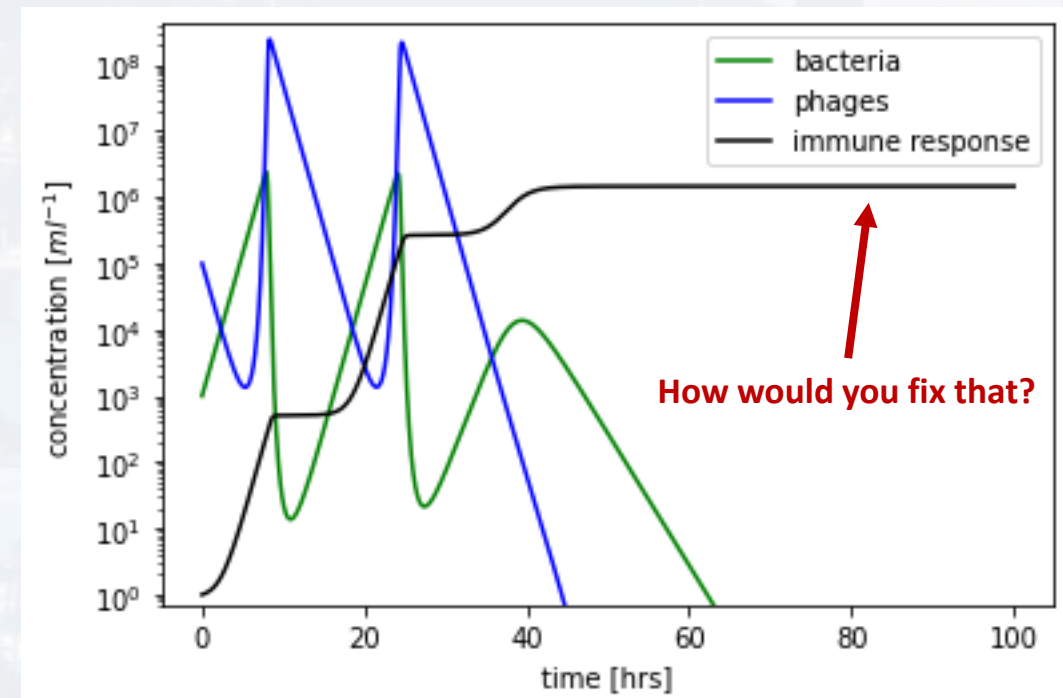
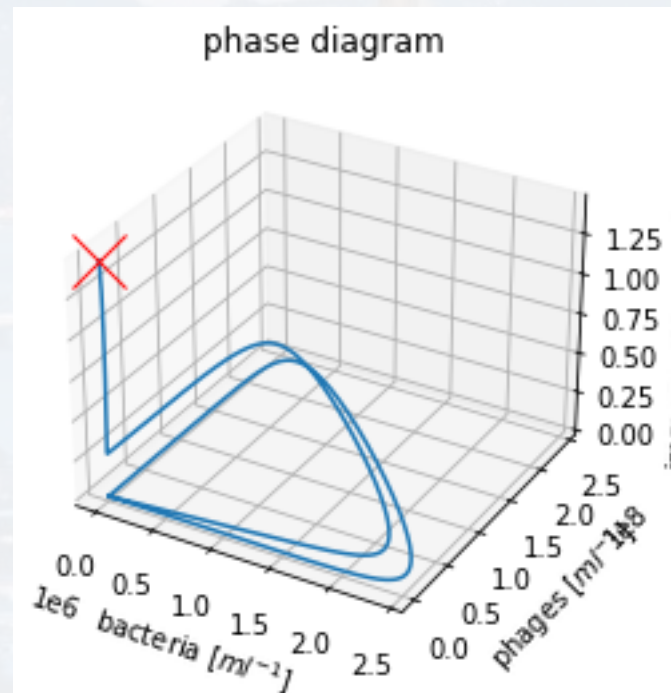


run:

```
SolvePhageTherapy(Init, t_span, rates)
```

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Thank you for your attention!

