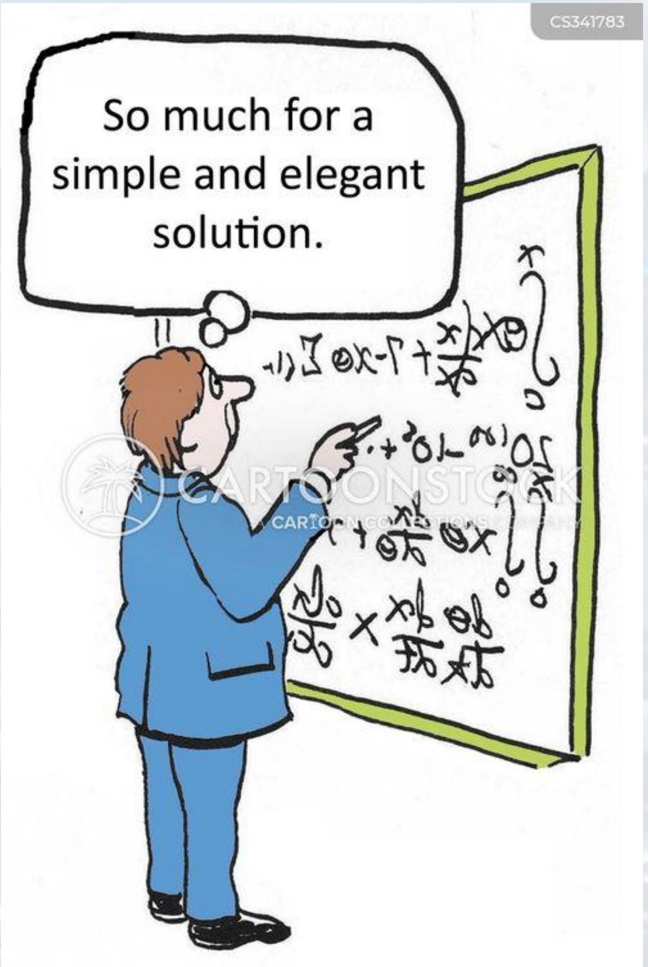
Berkeley
UNIVERSITY OF CALIFORNIA

M. Hohle:

Physics 77: Introduction to Computational Techniques in Physics



Introduction to Computational Techniques in Physics: syllabus

Week	Date	Topic
1	June 12th	Programming Environment & UIs for Python, Programming Fundamentals
2	*June 19th*	Basic Types in Python
3	June 26th	Parsing, Data Processing and File I/O, Visualization
4	July 3rd	Functions, Map & Lambda
5	July 10th	Random Numbers & Probability Distributions, Interpreting Measurements
6	July 17th	Numerical Integration and Differentiation
7	July 24th	Root finding, Interpolation
8	**July 31st**	Systems of Linear Equations, **Ordinary Differential Equations (ODEs)**
9	Aug 7th	Stability of ODEs, Examples
10	Aug 14th	Final Project Presentations

ordinary differential equation:

- **total** derivative → *ordinary* $\frac{d^k f(x)}{dx^k}$ $k \in \mathbb{N}$

- of **n-th** order → *n = max(k)*

- **non-linear** → *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

let's start simple:

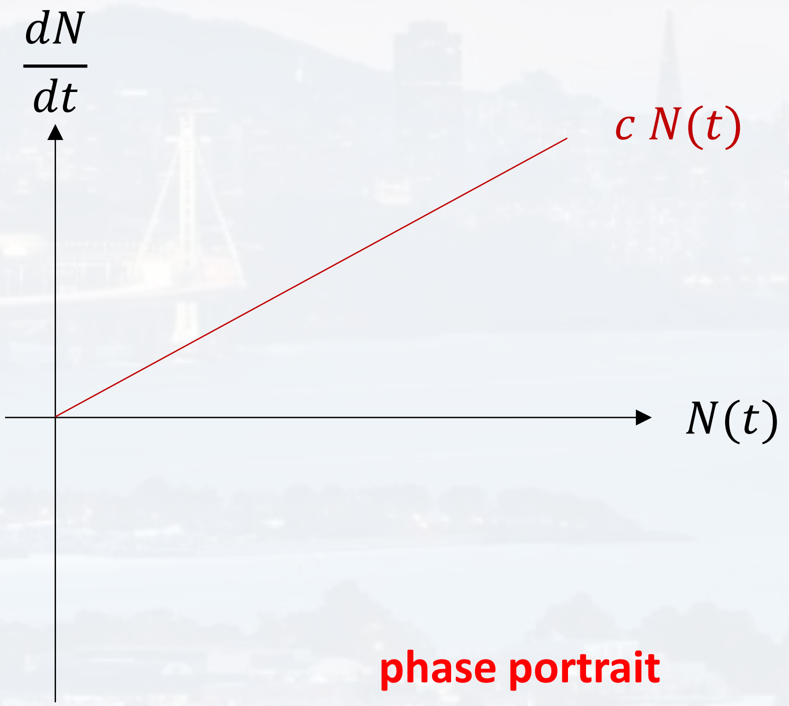
constant relative change per time step

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

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

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

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



phase portrait

let's start simple:

We want the model to have a limited carrying capacity κ

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

For $t \rightarrow \infty$ the island can only feed $N_{eq} = \kappa$ cows

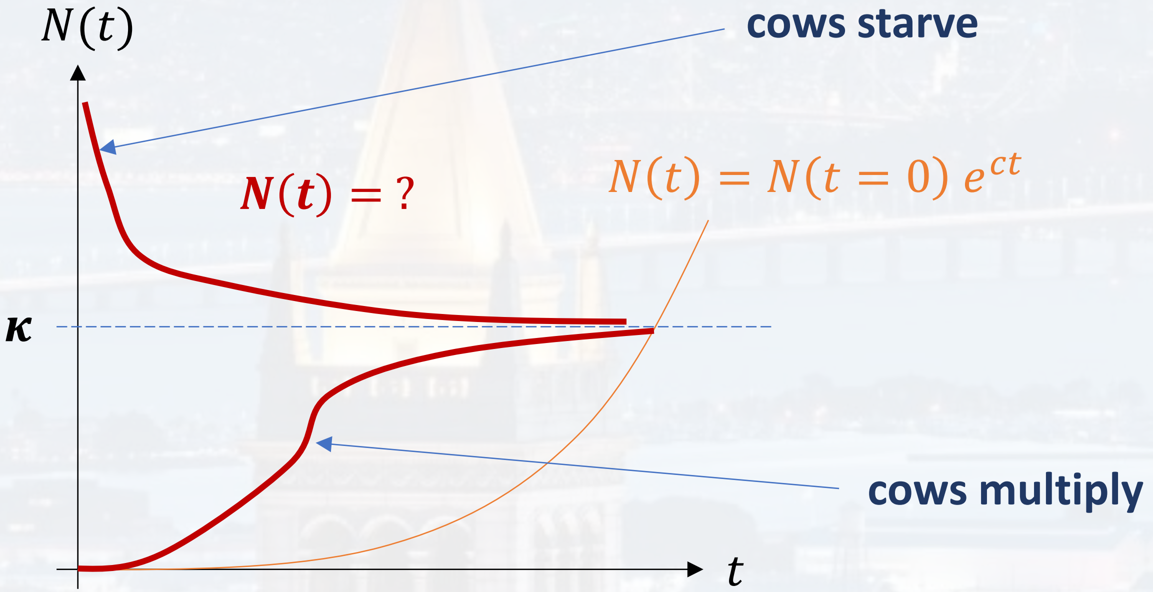
κ: carrying capacity

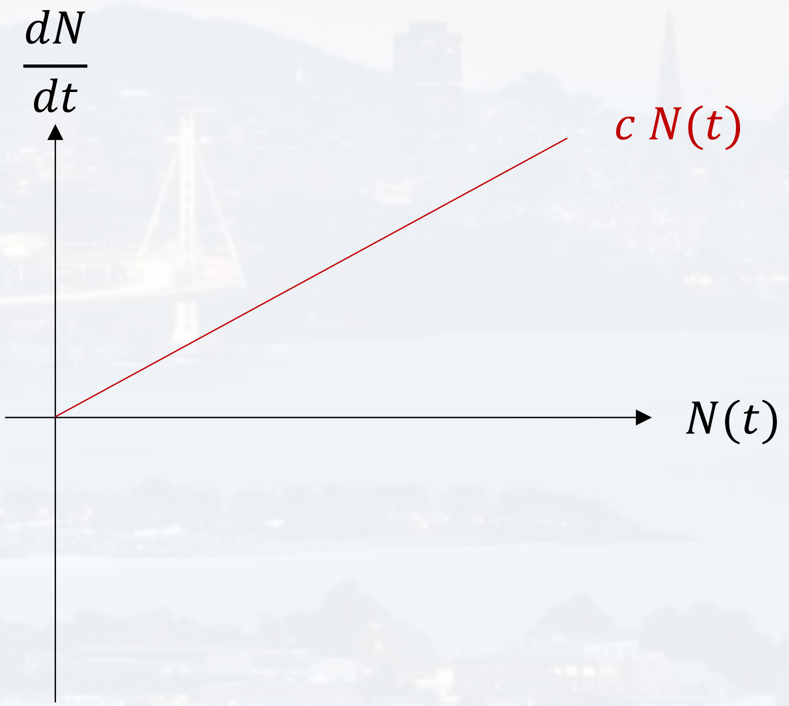
How do we model that?

let's start simple:

We want the model to have a limited **carrying capacity κ**

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

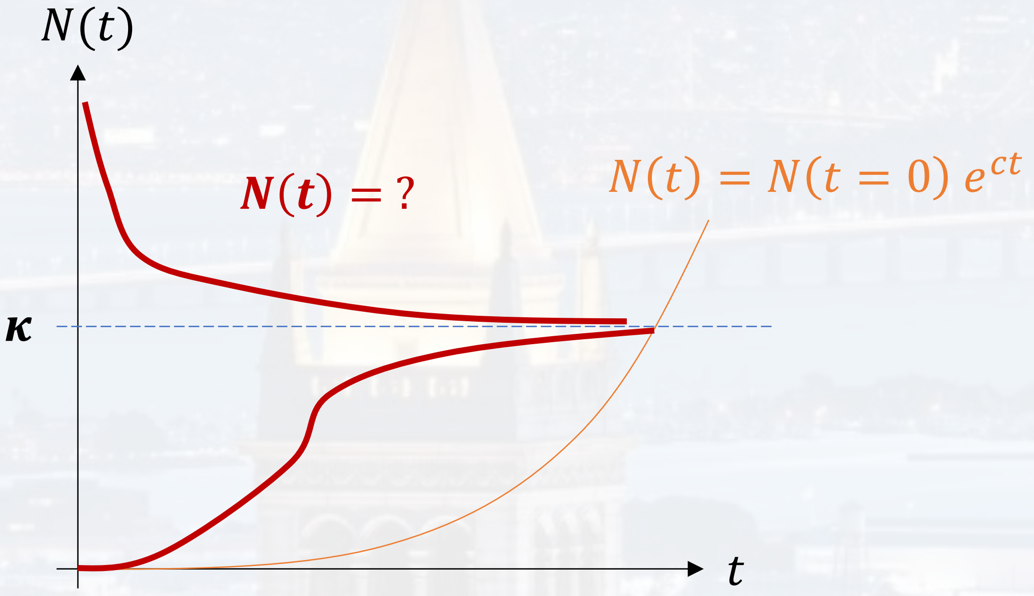


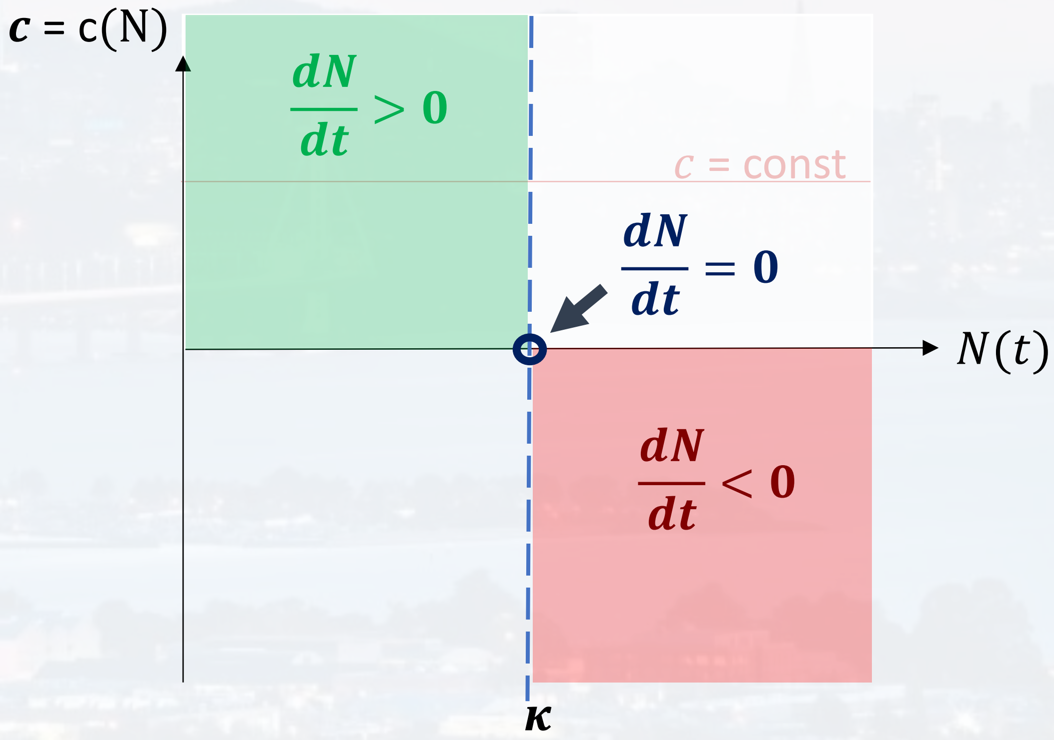


<u>let's start simple:</u>

We want the model to have a limited carrying capacity $\boldsymbol{\kappa}$

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





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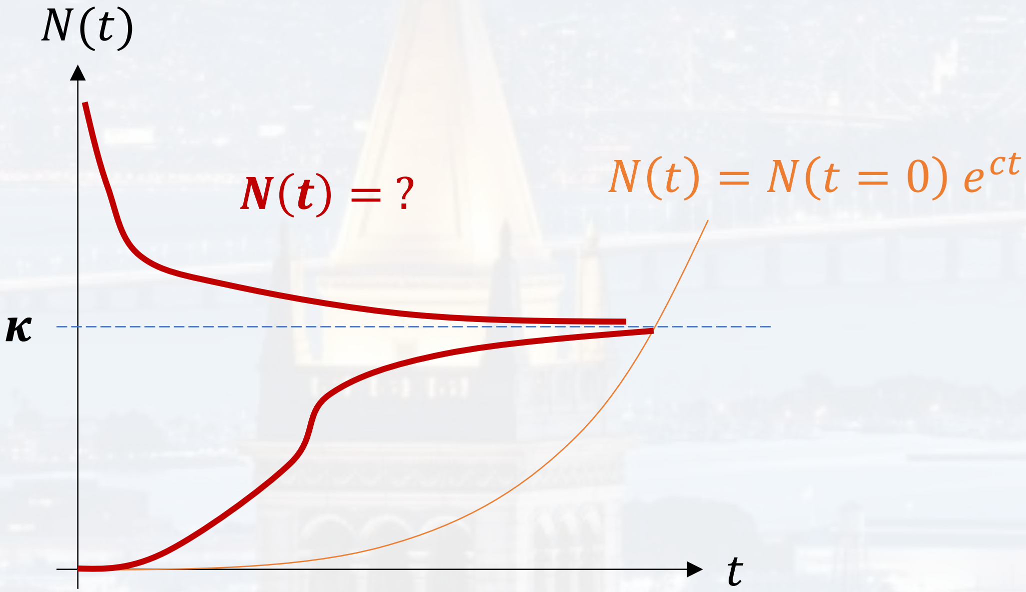

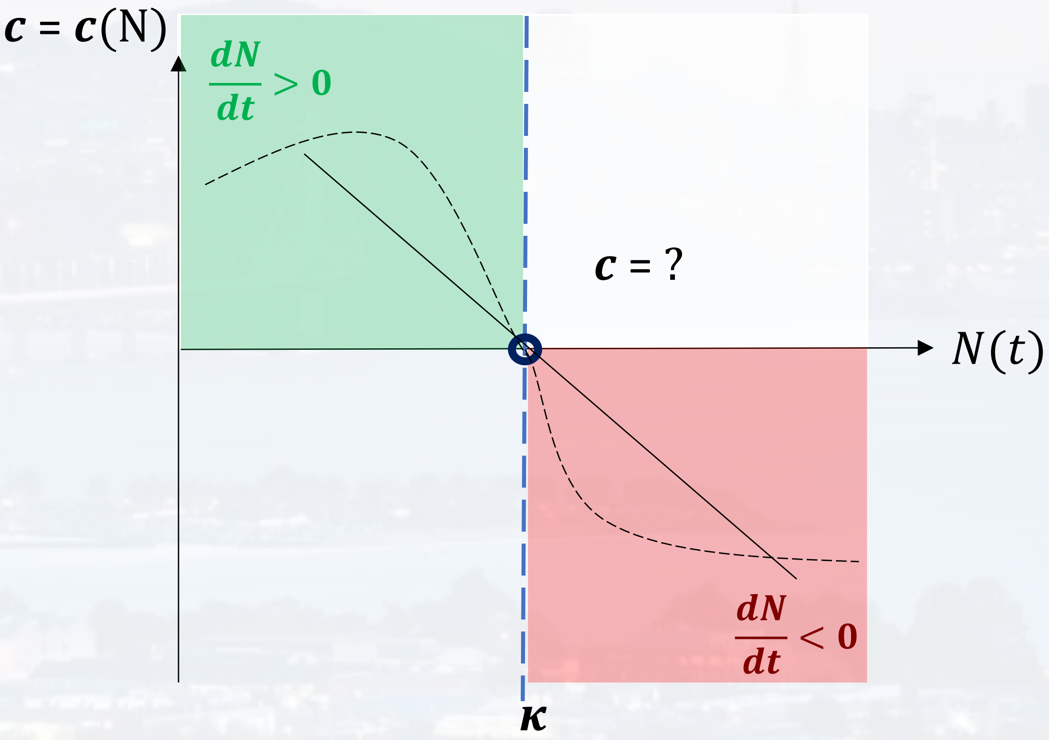

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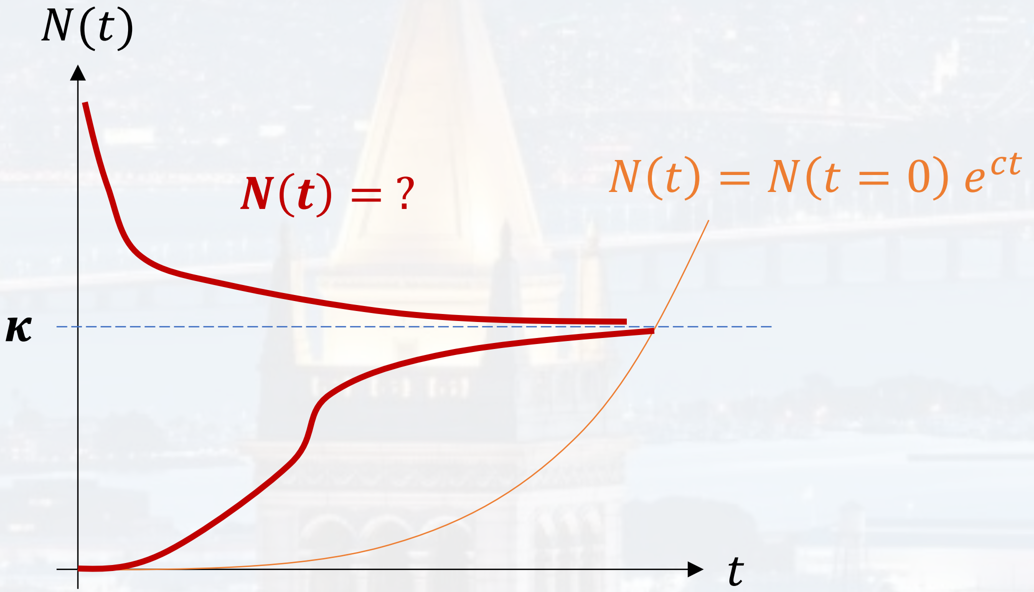
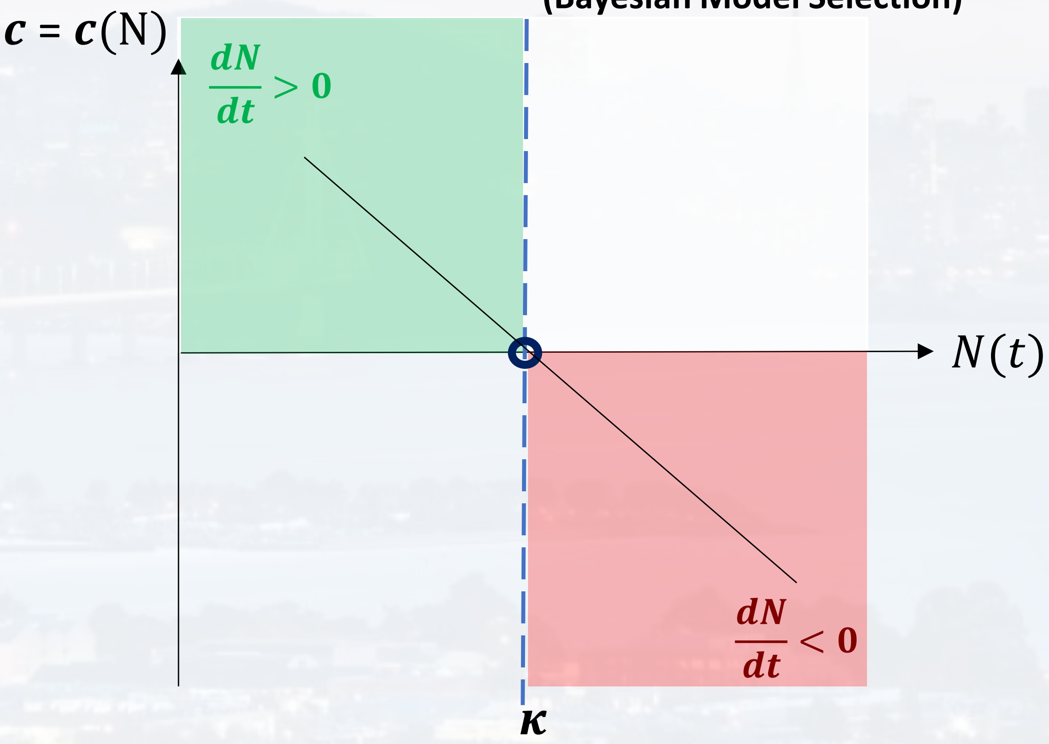
$$\frac{dN}{N} = c\,dt$$

Occam's razor:

prefer simple model
(Bayesian Model Selection)





let's start simple:

We want the model to have a limited carrying capacity $\boldsymbol{\kappa}$

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

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

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

$$c(0) = c_0$$

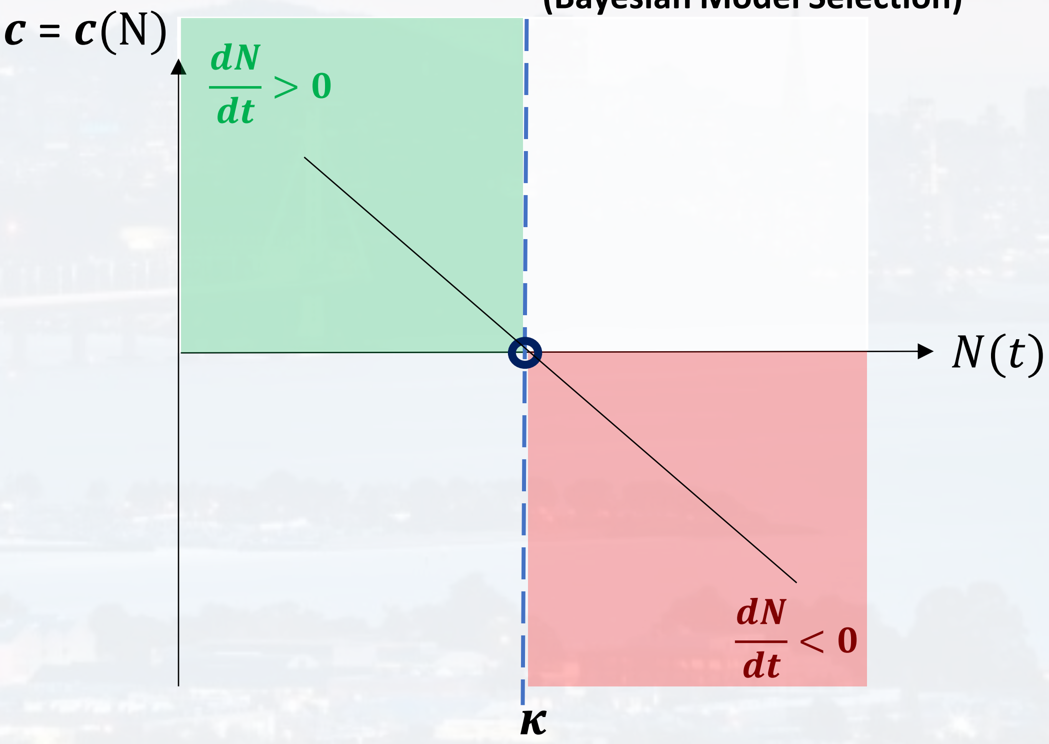
$$c(N) = c_0\left(1 - \frac{1}{\kappa}N\right)$$

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

Verhulst Equation

Occam's razor:

prefer simple model
(Bayesian Model Selection)



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

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Verhulst Equation

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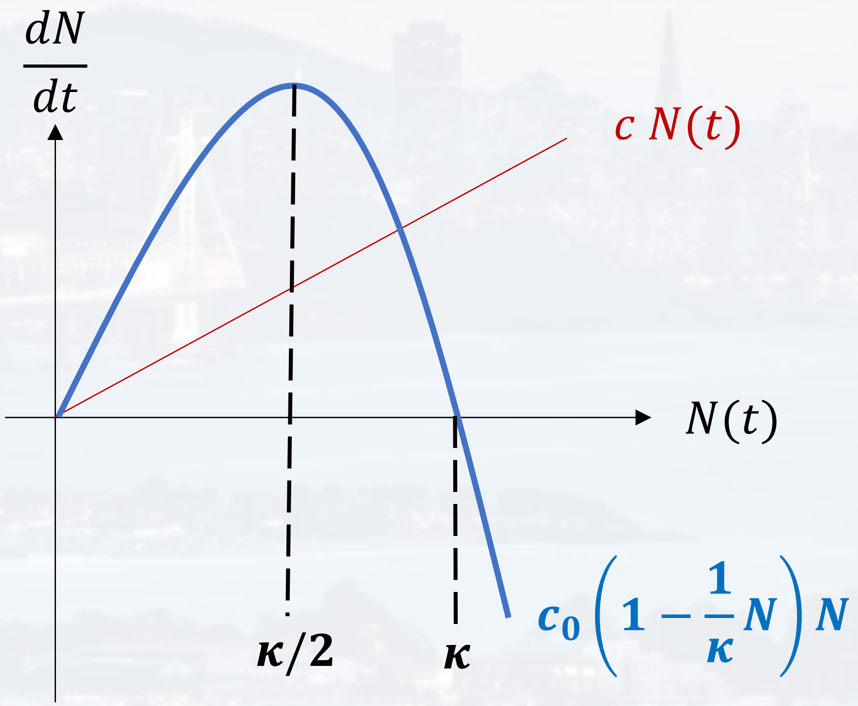

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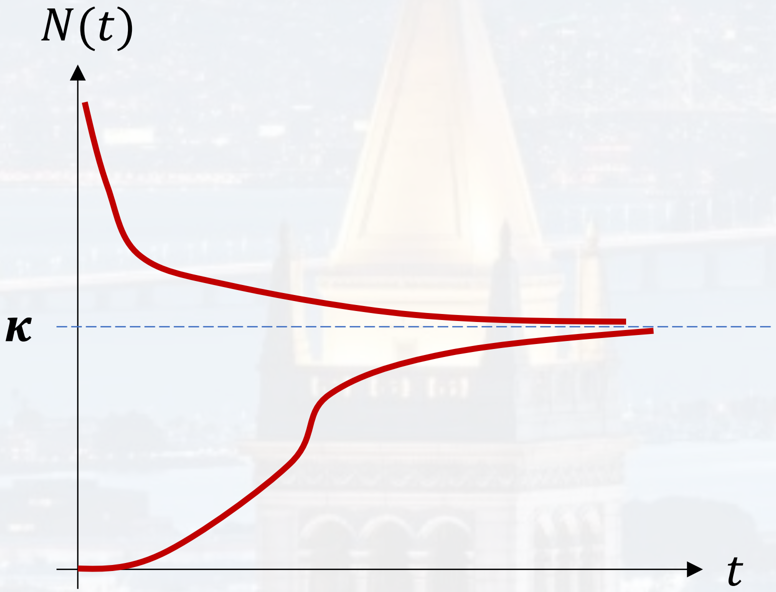
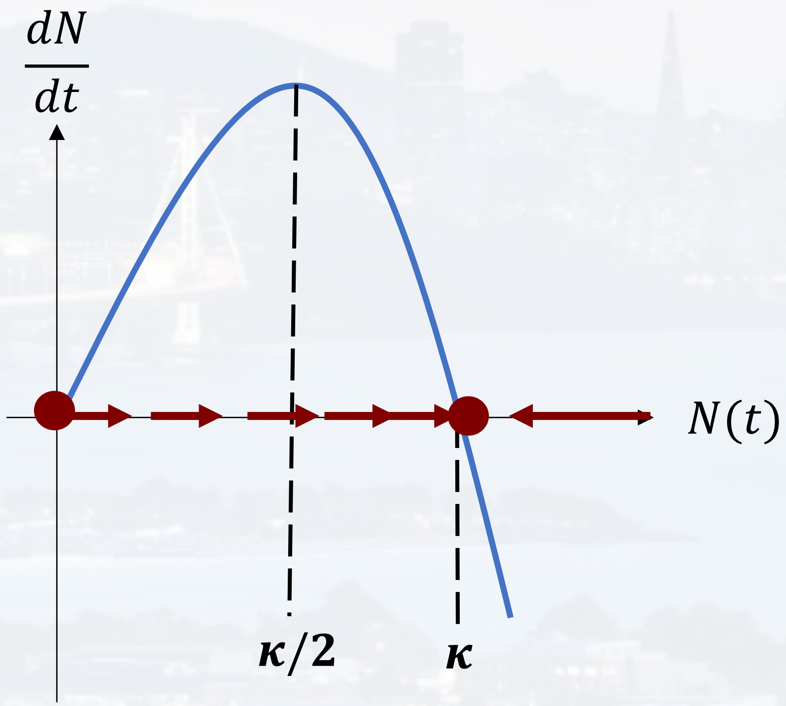
We want the model to have a limited carrying capacity κ

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

Verhulst Equation





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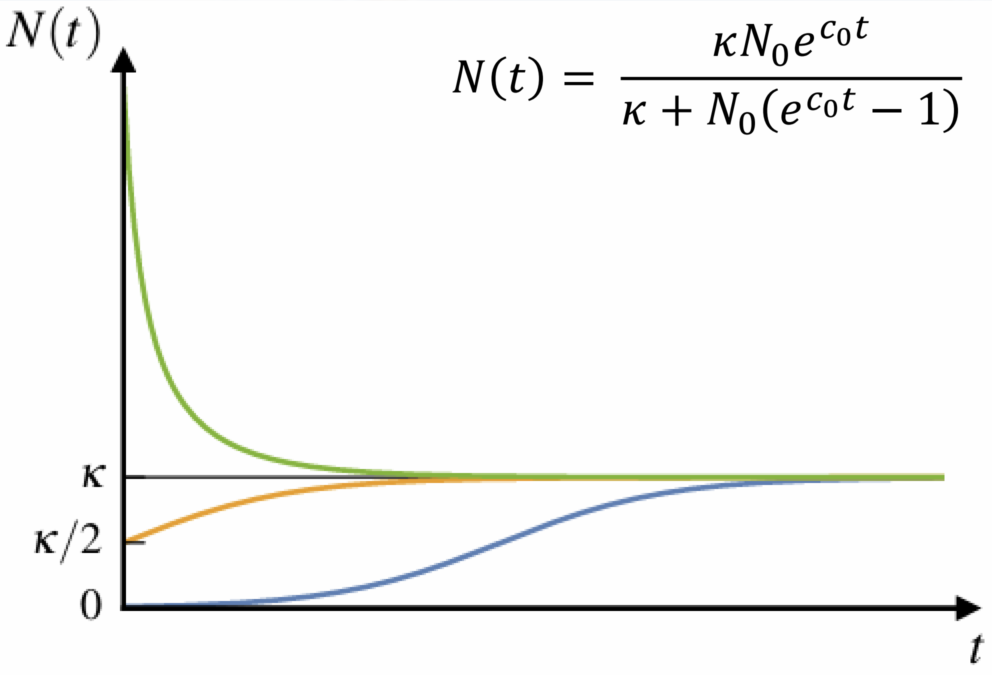
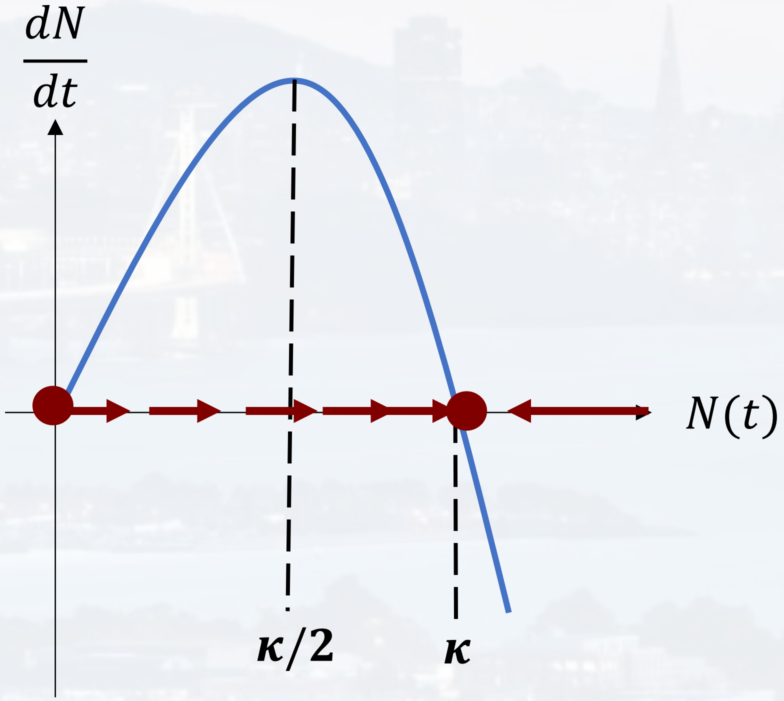
$$\frac{dN}{dt} = c_0\left(1 - \frac{1}{\kappa}N\right)N$$

Verhulst Equation





let's start simple:

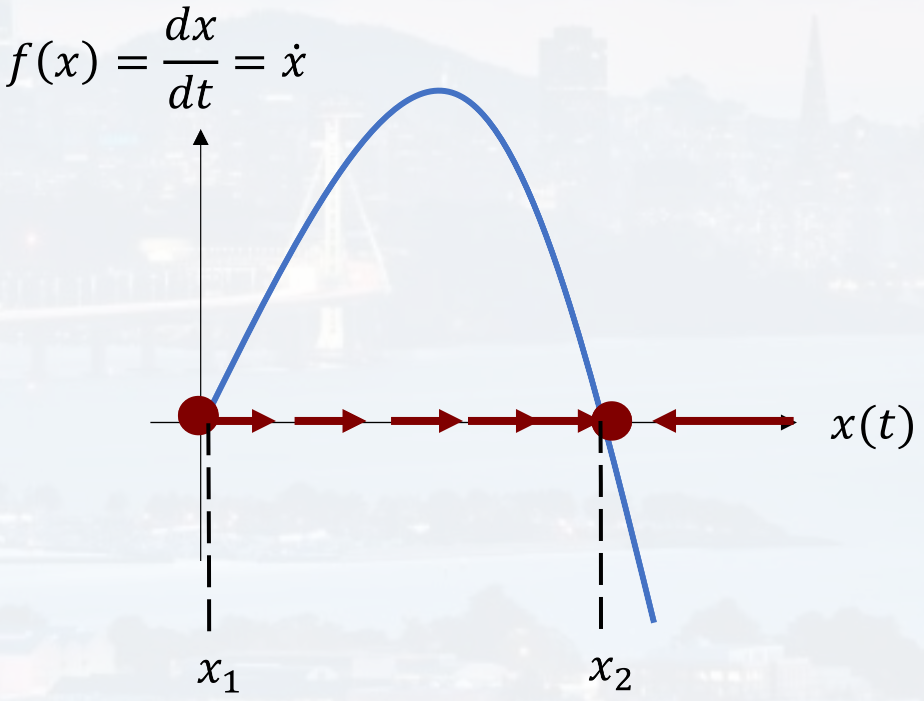
We want the model to have a limited carrying capacity $\boldsymbol{\kappa}$

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

Verhulst Equation

x_1, x_2 fixed points

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



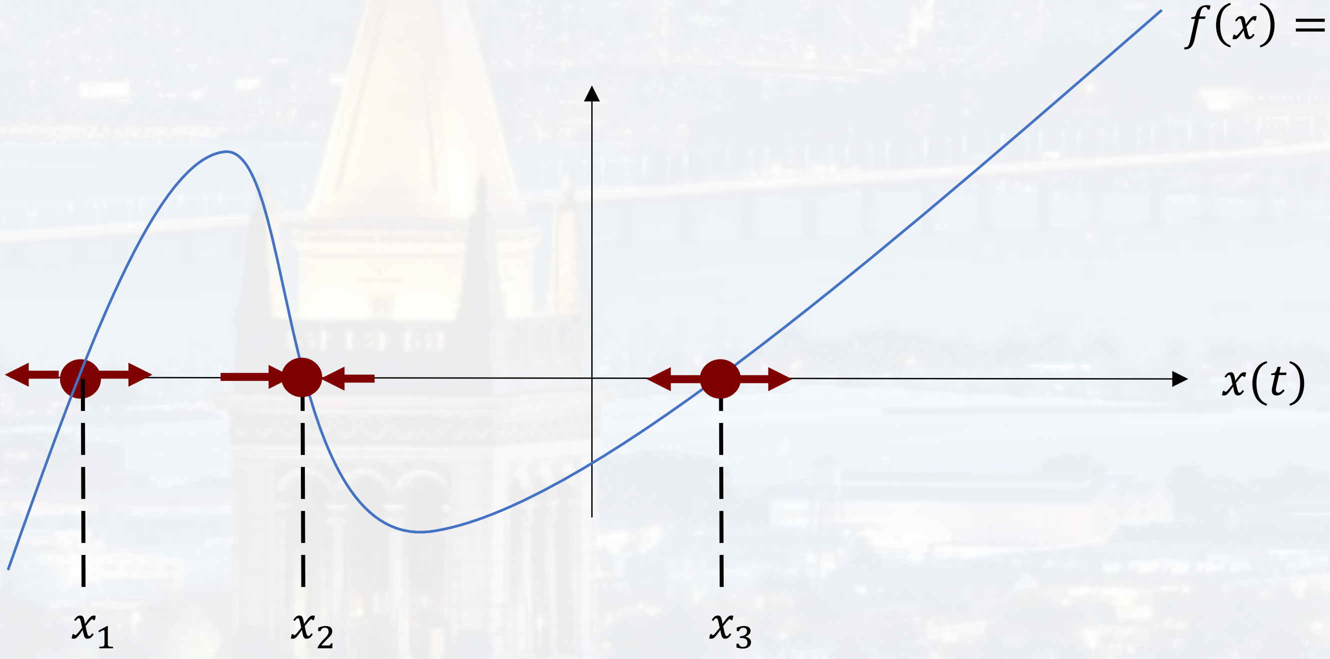
fixed points x^*

x_1: repeller → unstable
x_3: repeller → unstable

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

x_2: attractor → stable

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



fixed points x^*

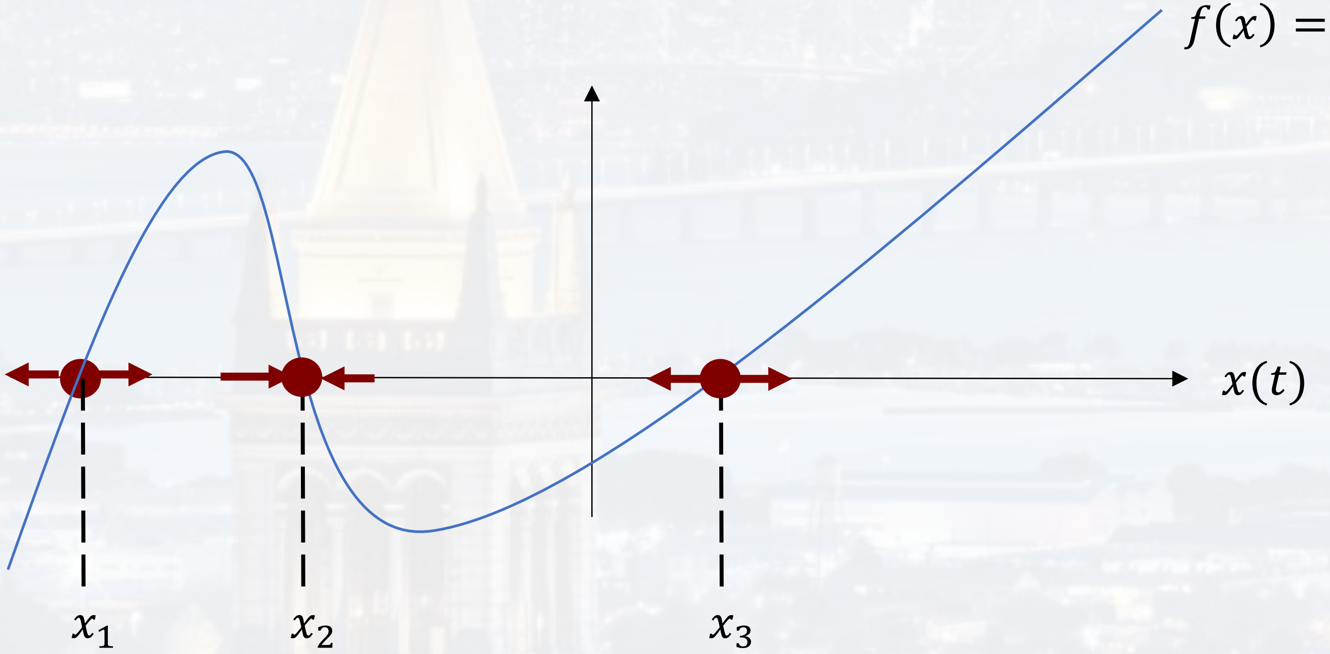
small perturbation $\varepsilon(t)$

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

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

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

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



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

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

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

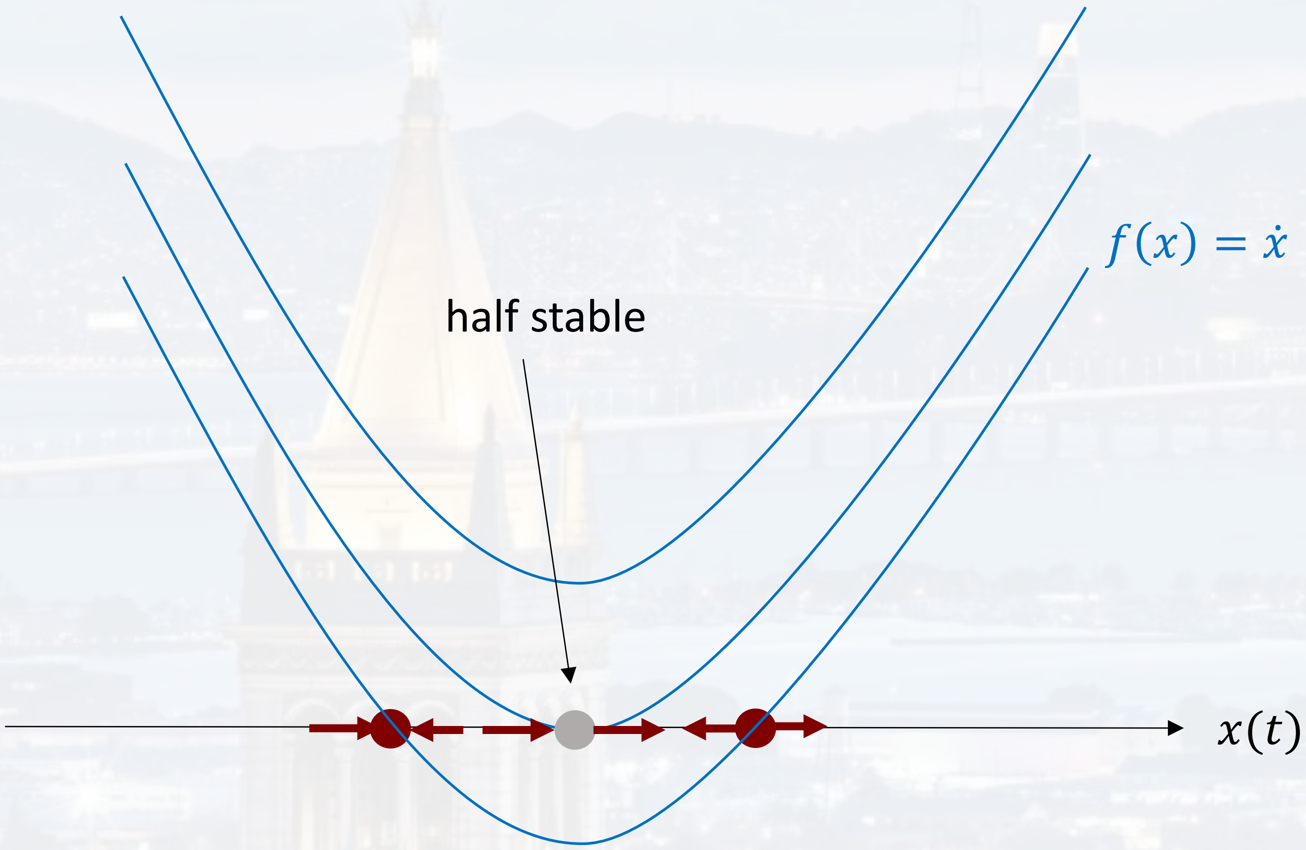
fixed points x^*

small perturbation $\varepsilon(t)$

$$\varepsilon(t) = \varepsilon_0\, e^{\frac{df(x)}{dx}|_{x=x^*}\, t} \qquad \text{time scale } \tau = \frac{1}{\frac{df(x)}{dx}|_{x=x^*}}$$

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

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



fixed points x^*

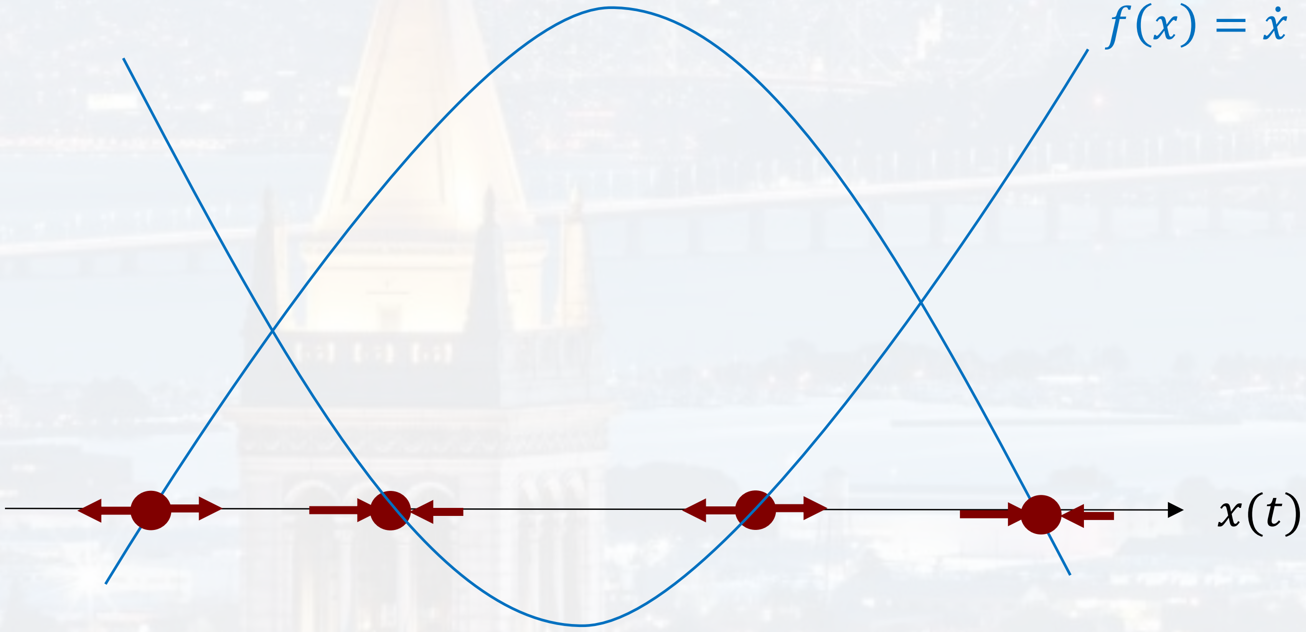
small perturbation $\varepsilon(t)$

$$\varepsilon(t) = \varepsilon_0 \, e^{\frac{df(x)}{dx}|_{x=x^*} t} \qquad \text{time scale } \tau = \frac{1}{\frac{df(x)}{dx}|_{x=x^*}}$$

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

$$f(x) = \boldsymbol{a}x^2 + \boldsymbol{b}x + \boldsymbol{c}$$

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



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

2D system

$$f(x,y) = \dot{x} \qquad \dot{x} = -x + a\,y + x^2 y$$

a, b >0

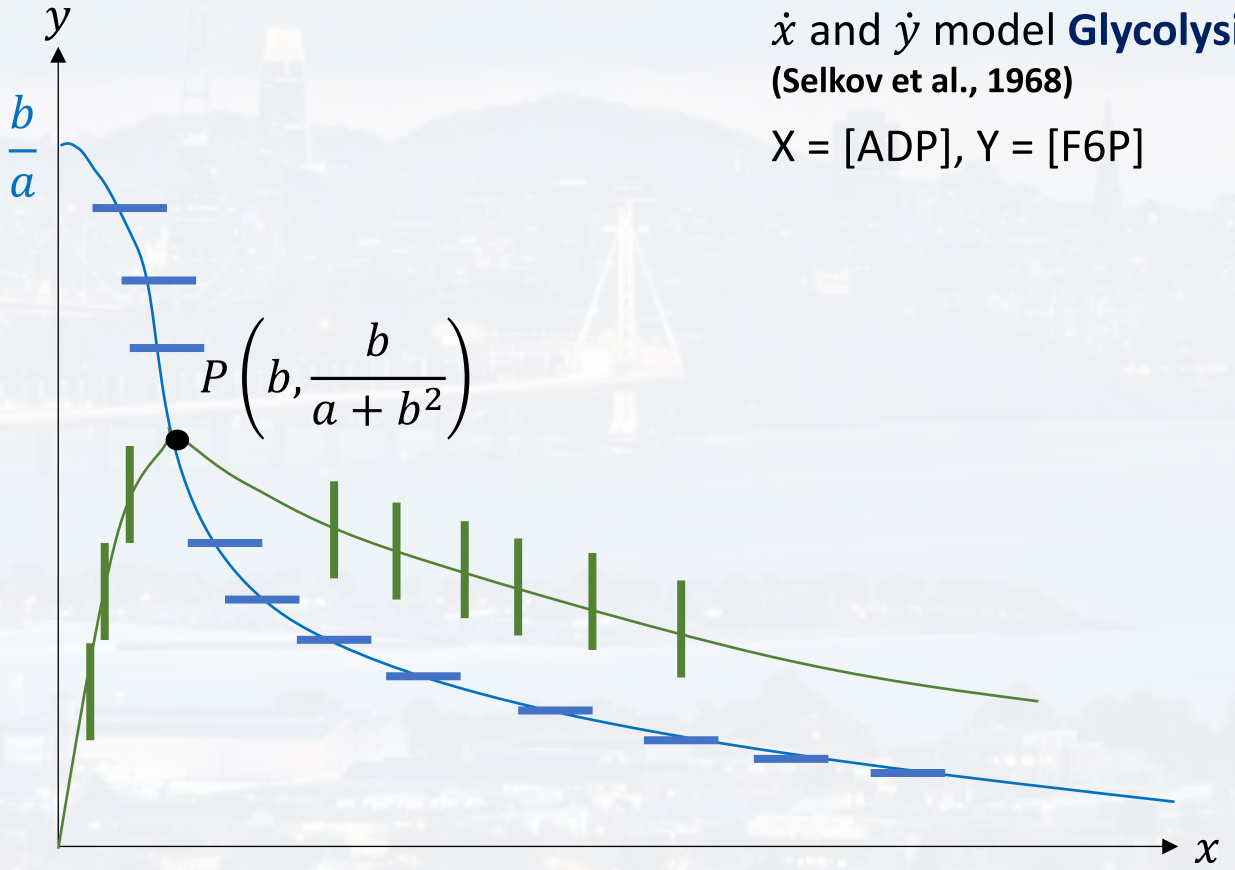
$$g(x,y) = \dot{y} \qquad \dot{y} = b - a\,y - x^2 y$$

non-linear, coupled ODEs

null clines

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

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



$\dot{x}$ and $\dot{y}$ model **Glycolysis**

(Selkov et al., 1968)

X = [ADP], Y = [F6P]

Find out which way the system moves!

2D system

$f(x,y) = \dot{x}$ $\qquad \dot{x} = -x + a\,y + x^2 y$ $\qquad$ a, b >0

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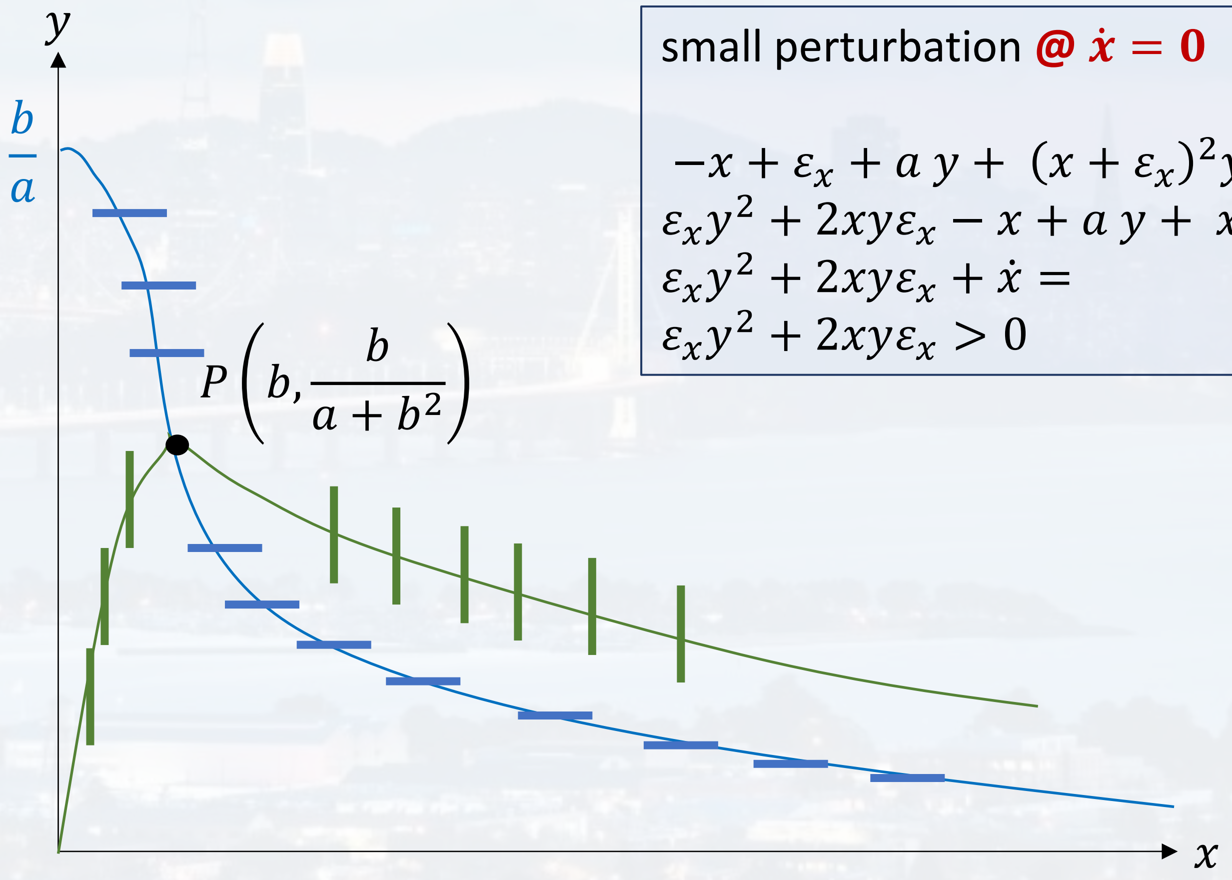

small perturbation $@\ \dot{x} = 0$

$$-x + \varepsilon_x + a\,y + (x + \varepsilon_x)^2 y =$$
$$\varepsilon_x y^2 + 2xy\varepsilon_x - x + a\,y + x^2 y =$$
$$\varepsilon_x y^2 + 2xy\varepsilon_x + \dot{x} =$$
$$\varepsilon_x y^2 + 2xy\varepsilon_x > 0$$

Find out which way the system moves!

2D system

$$f(x,y) = \dot{x} \qquad \dot{x} = -x + a\,y + x^2 y \qquad \text{a, b >0}$$

$$g(x,y) = \dot{y} \qquad \dot{y} = b - a\,y - x^2 y$$

null clines

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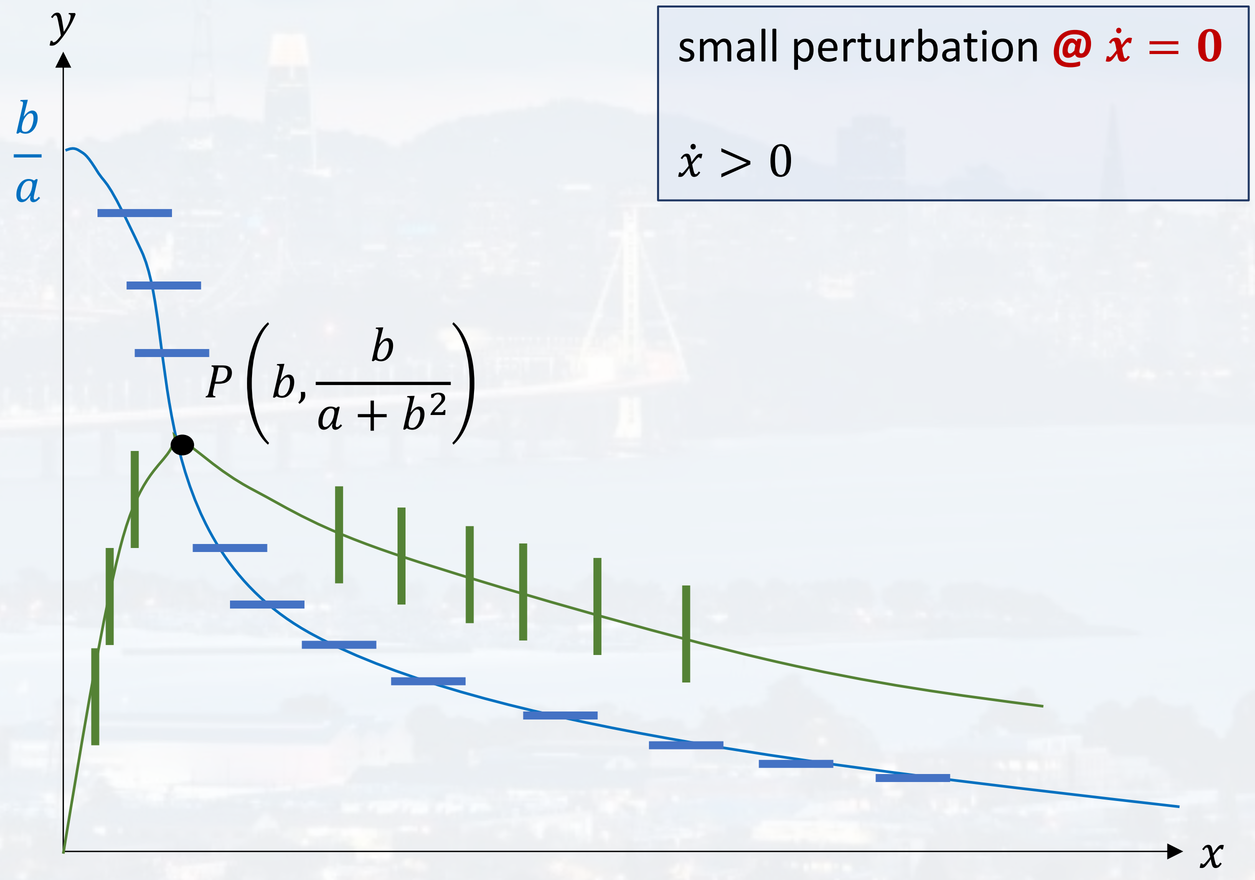


small perturbation @ $\dot{x} = 0$

$\dot{x} > 0$

Find out which way the system moves!

2D system

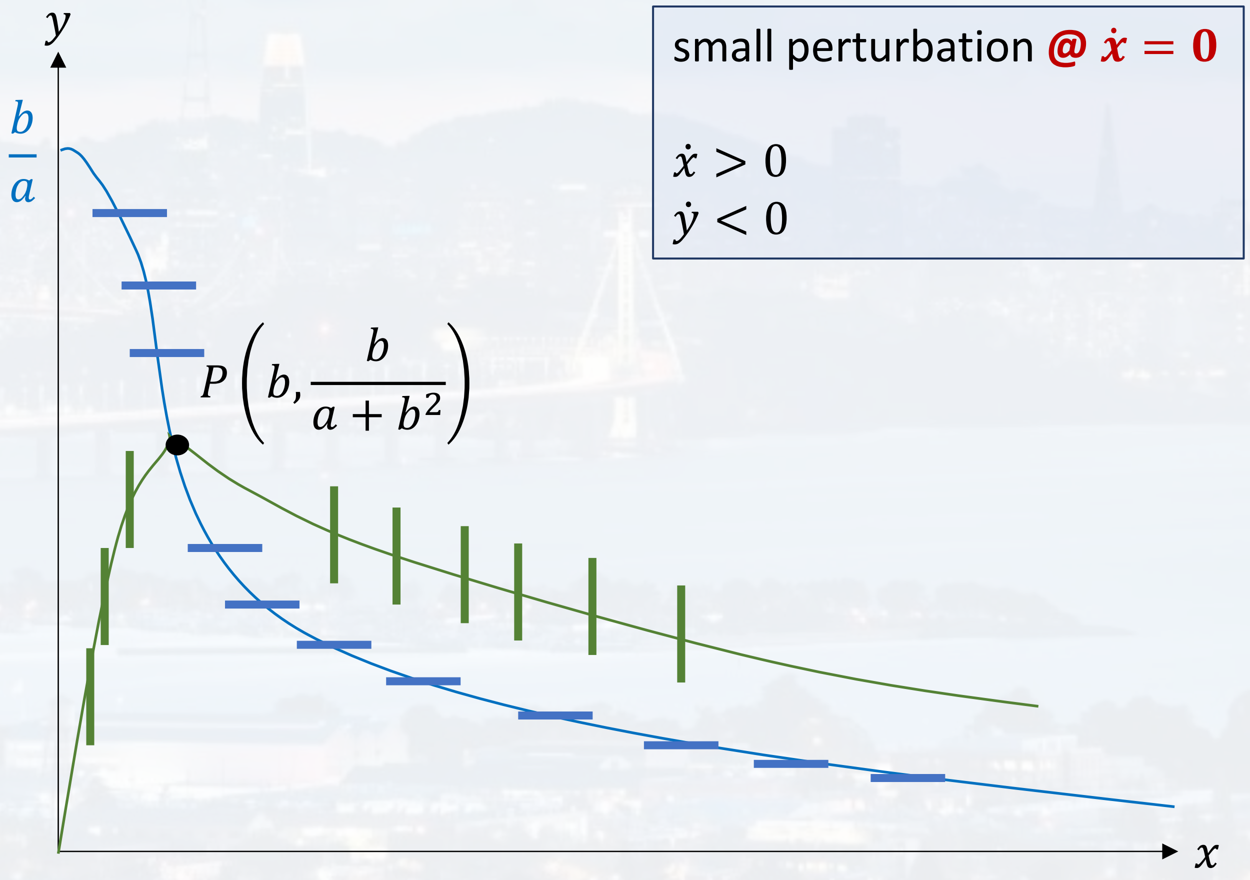
$f(x, y) = \dot{x}$ $\qquad$ $\dot{x} = -x + a\,y + x^2 y$ $\qquad$ a, b >0

$g(x, y) = \dot{y}$ $\qquad$ $\dot{y} = b - a\,y - x^2 y$

null clines

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

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



small perturbation @ $\dot{x} = 0$

$\dot{x} > 0$
$\dot{y} < 0$

Find out which way the system moves!

2D system

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

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

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

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a, b >0

null clines

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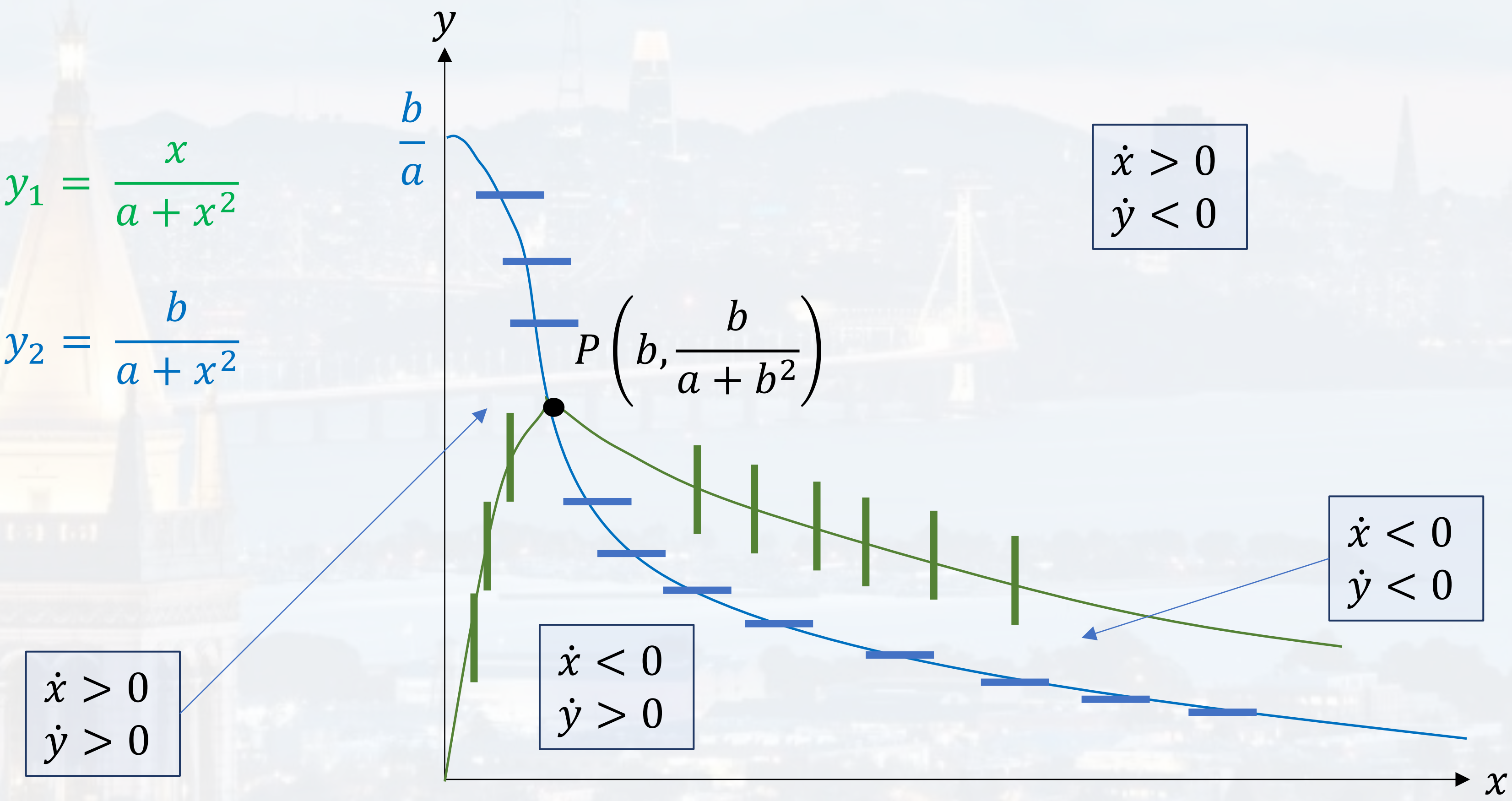

2D system

$$f(x,y) = \dot{x} \qquad \dot{x} = -x + a\,y + x^2 y \qquad \text{a, b > 0}$$

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null clines

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

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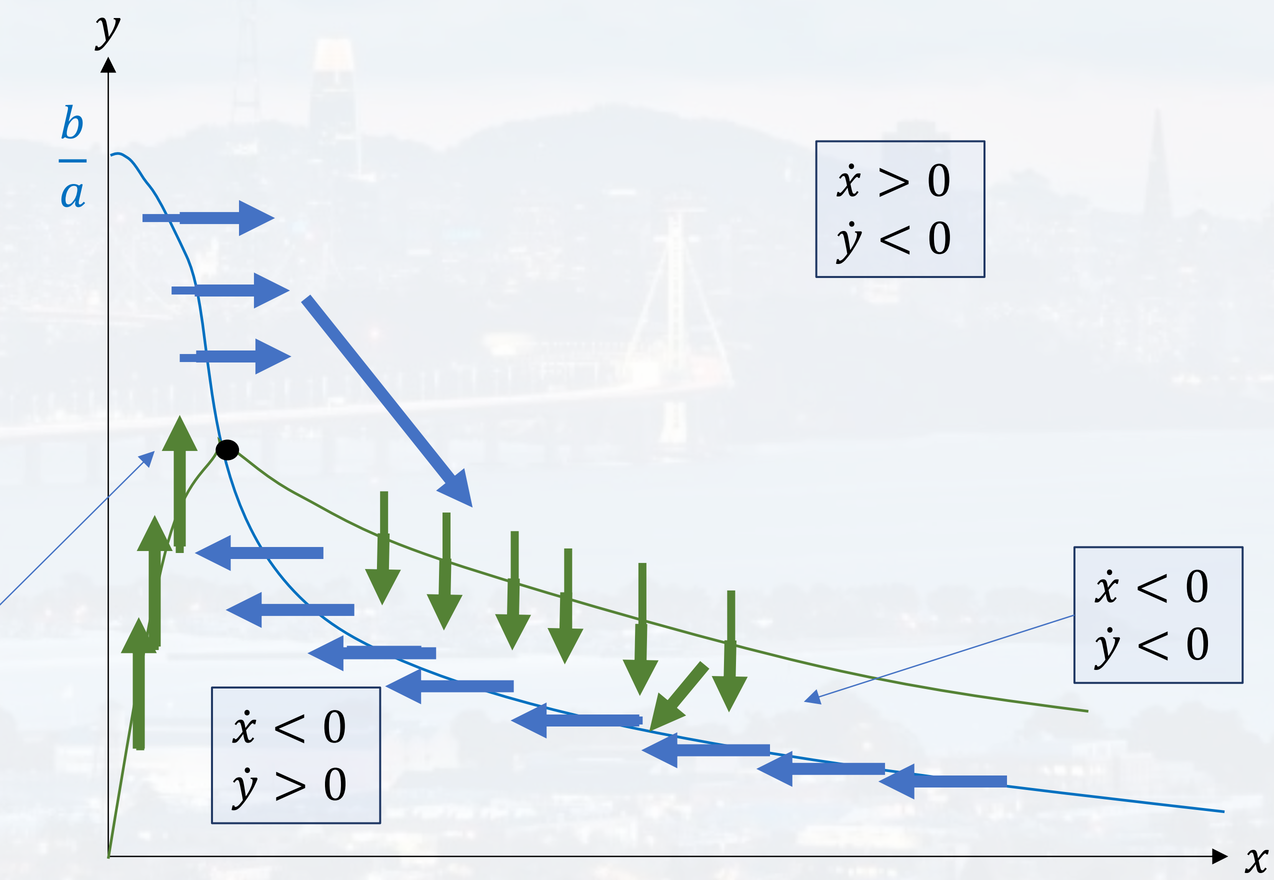

2D system

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

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$\dot{x} = -x + a\,y + x^2 y$ a, b >0

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

null clines

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

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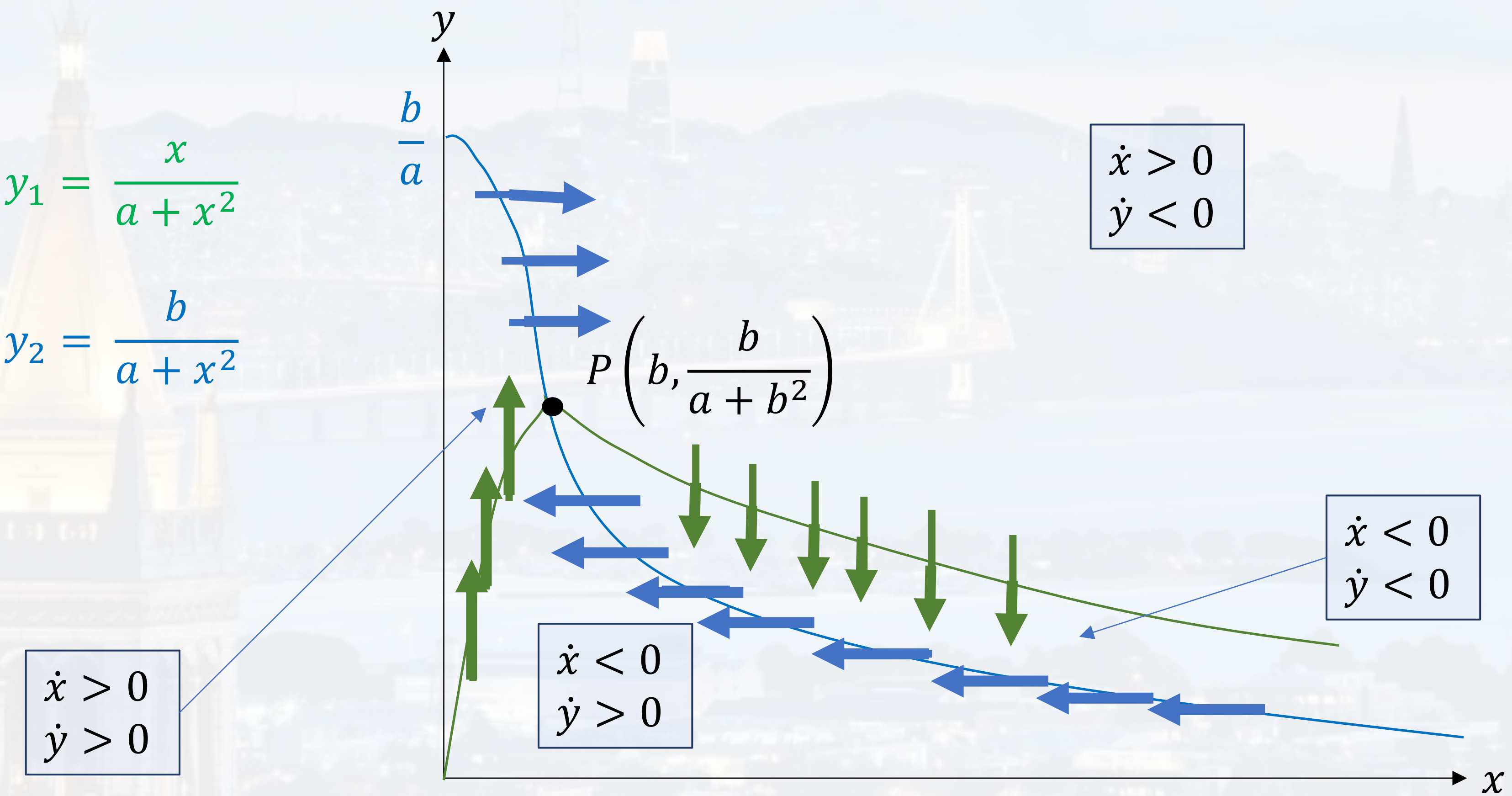

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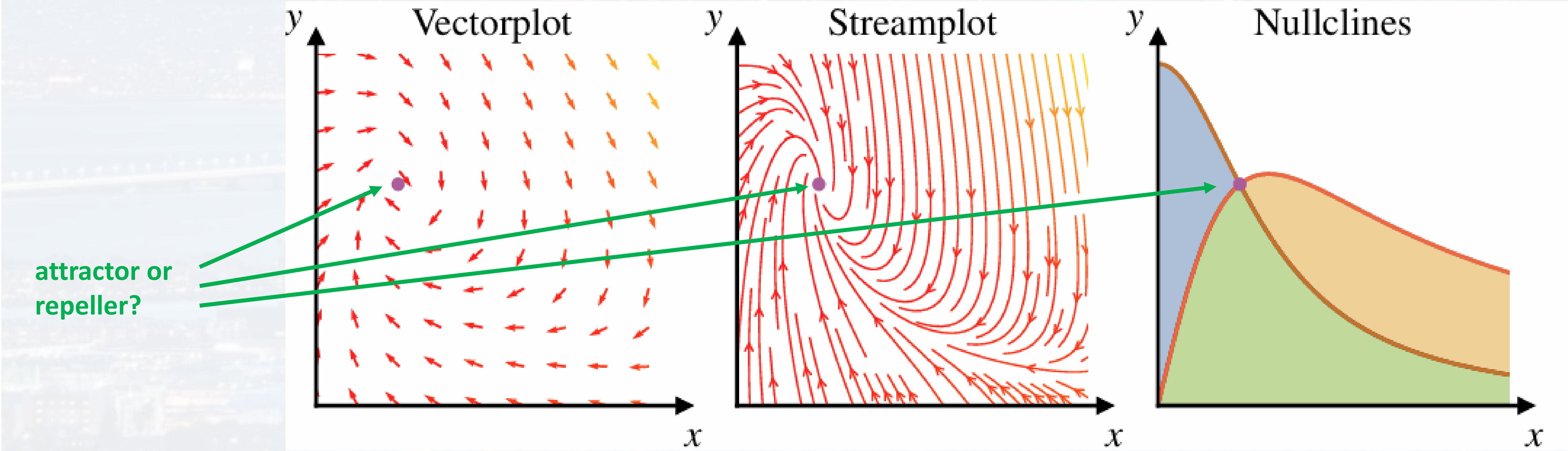
$$g(x,y) = \dot{y} \qquad \dot{y} = b - a\,y - x^2 y \qquad \text{non-linear, coupled ODEs}$$

$\dot{x} = 0 \rightarrow \quad y_1 = \frac{x}{a + x^2}$ $\qquad \dot{y} = 0 \rightarrow \quad y_2 = \frac{b}{a + x^2}$



2D system

$f(x,y) = \dot{x}$ $\quad\quad$ $\dot{x} = -x + a\,y + x^2 y$ $\quad\quad$ a, b >0

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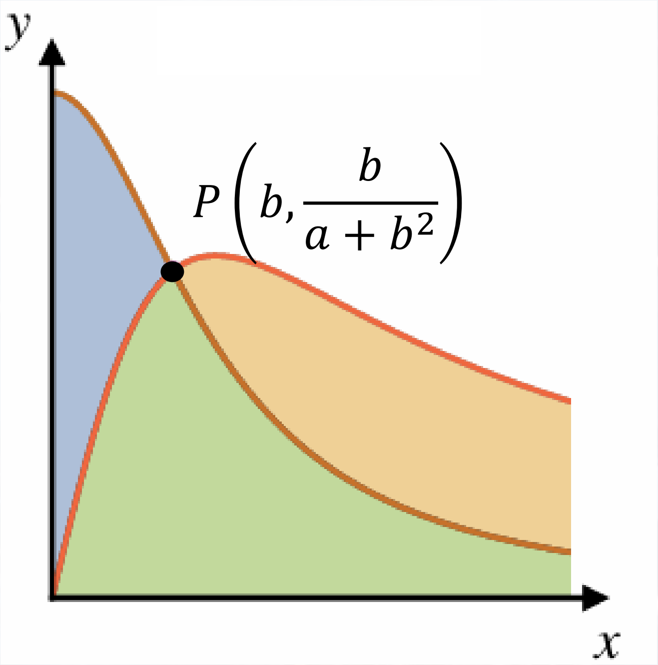
stability of P:



$$\underbrace{f(x^* + \varepsilon_x, y^* + \varepsilon_y)}_{\frac{d\,\varepsilon_x(t)}{dt}} \approx \underbrace{f(x^*, y^*)}_{=0} + \underbrace{\frac{\partial f(x,y)}{\partial x}|_{x^*,y^*}}_{\alpha} \varepsilon_x + \underbrace{\frac{\partial f(x,y)}{\partial y}|_{x^*,y^*}}_{\beta} \varepsilon_y$$

$$\underbrace{g(x^* + \varepsilon_x, y^* + \varepsilon_y)}_{\frac{d\,\varepsilon_y(t)}{dt}} \approx \underbrace{g(x^*, y^*)}_{=0} + \underbrace{\frac{\partial g(x,y)}{\partial x}|_{x^*,y^*}}_{\gamma} \varepsilon_x + \underbrace{\frac{\partial g(x,y)}{\partial y}|_{x^*,y^*}}_{\delta} \varepsilon_y$$

$$\dot{\vec{\varepsilon}} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \vec{\varepsilon}$$

2D system

$f(x,y) = \dot{x}$ $\qquad \dot{x} = -x + a\,y + x^2 y$ $\qquad$ a, b >0

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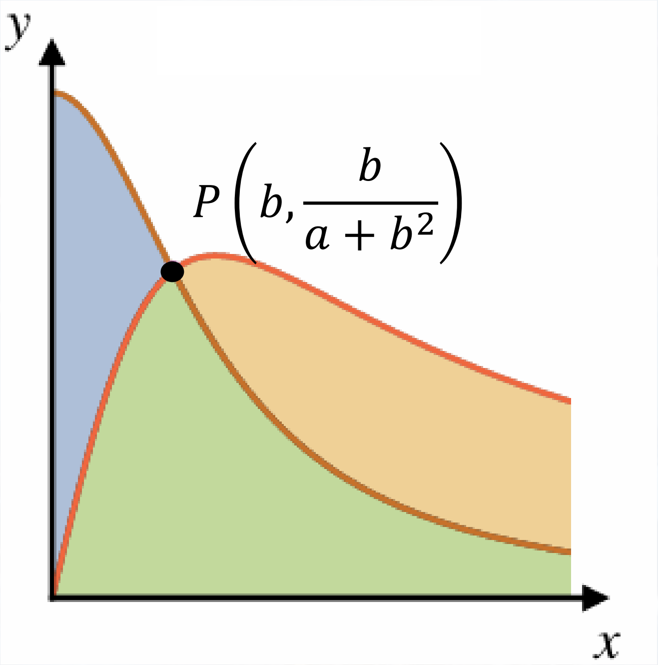
stability of P:



$$\dot{\vec{\varepsilon}} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \vec{\varepsilon} \qquad A = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \qquad \varepsilon(t) = \varepsilon_0\, e^{\frac{df(x)}{dx}|_{x=x^*}\, t}$$

$$\vec{\varepsilon}(t) = \vec{\varepsilon}(t=0)\, e^{\lambda t}$$ λ: eigenvalue of A

$$0 \overset{!}{=} det \begin{pmatrix} \alpha - \lambda & \beta \\ \gamma & \delta - \lambda \end{pmatrix} = \lambda^2 - (\alpha+\delta)\lambda + (\alpha\delta - \gamma\beta)$$

one can show that $\tau = \dfrac{b^4 + (2a-1)b^2 + a(1+a)}{a + b^2}$

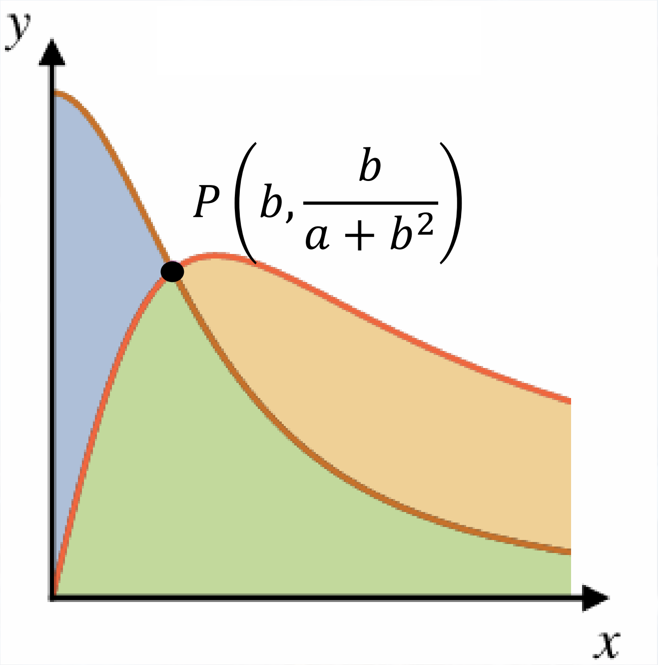
$\tau > 0$ P is a repeller
$\tau < 0$ P is an attractor

2D system

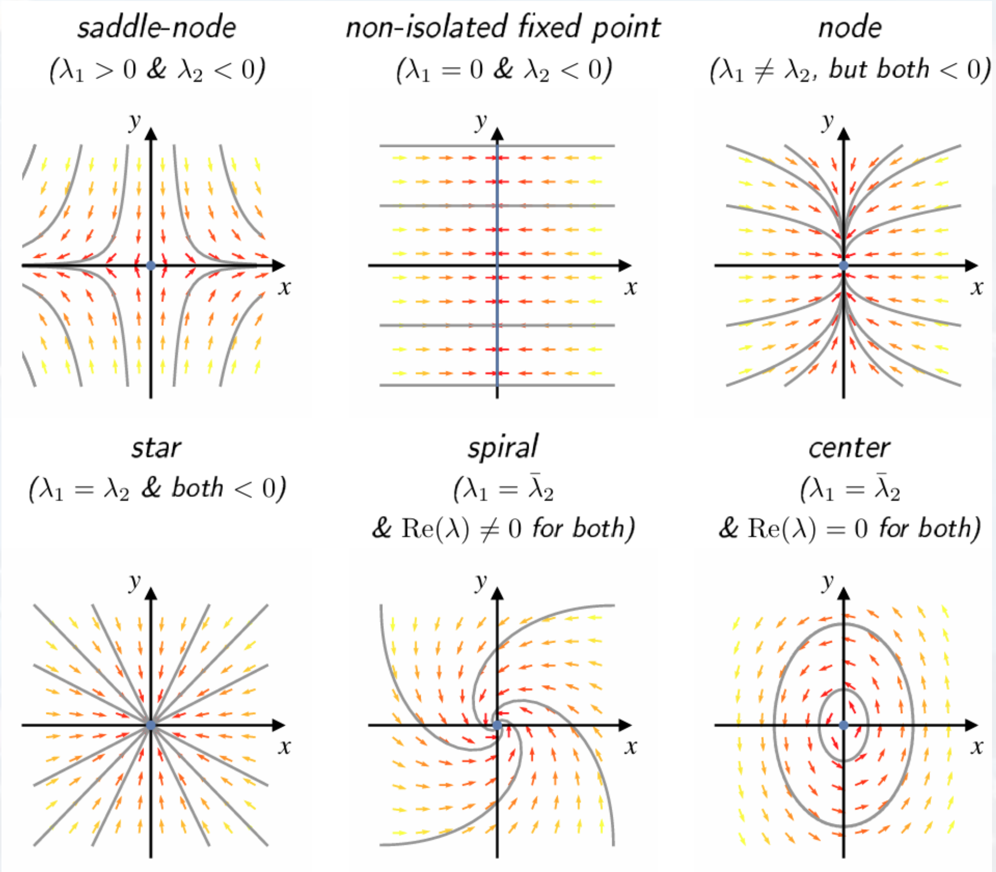
$$f(x,y) = \dot{x} \qquad \dot{x} = -x + a\,y + x^2 y \qquad \text{a, b >0}$$

$$g(x,y) = \dot{y} \qquad \dot{y} = b - a\,y - x^2 y \qquad \text{non-linear, coupled ODEs}$$

stability of P: $\vec{\varepsilon}(t) = \vec{\varepsilon}(t=0)\, e^{\lambda t}$



attractor: real part of all eigenvalues has to be negative!



2D system

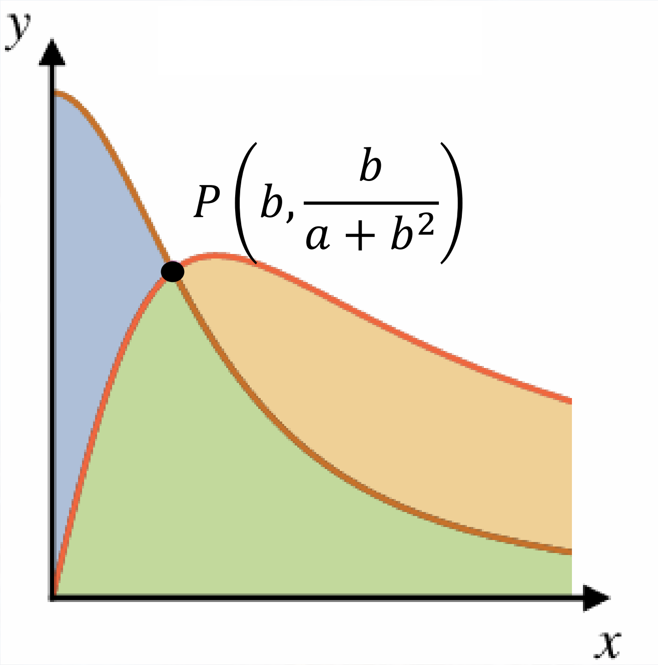
$$f(x,y) = \dot{x} \qquad \dot{x} = -x + a\,y + x^2 y$$

$$g(x,y) = \dot{y} \qquad \dot{y} = b - a\,y - x^2 y$$

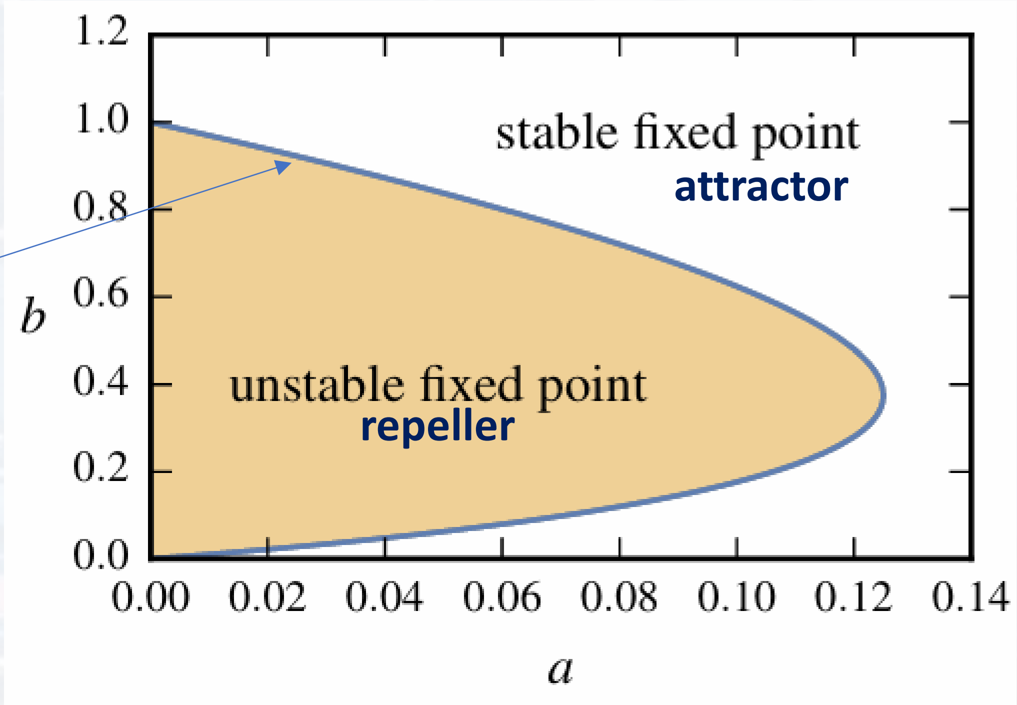
stability of P: $\vec{\varepsilon}(t) = \vec{\varepsilon}(t=0)\, e^{\lambda t}$ $\quad \tau = \dfrac{b^4 + (2a-1)b^2 + a(1+a)}{a + b^2}$

$\tau > 0$ **P is a repeller**

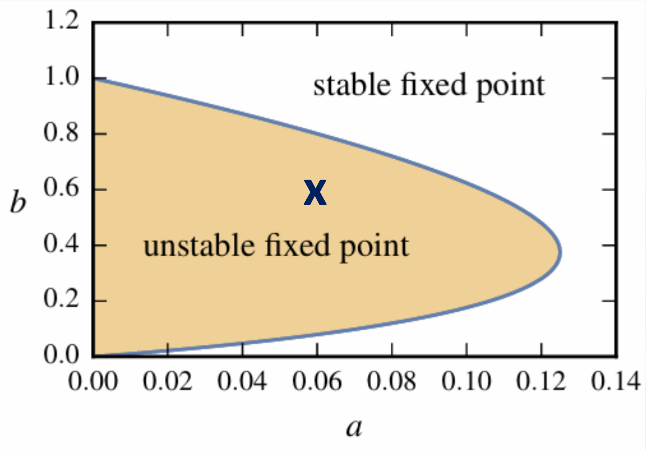
$\tau < 0$ **P is an attractor**



$\tau = 0$



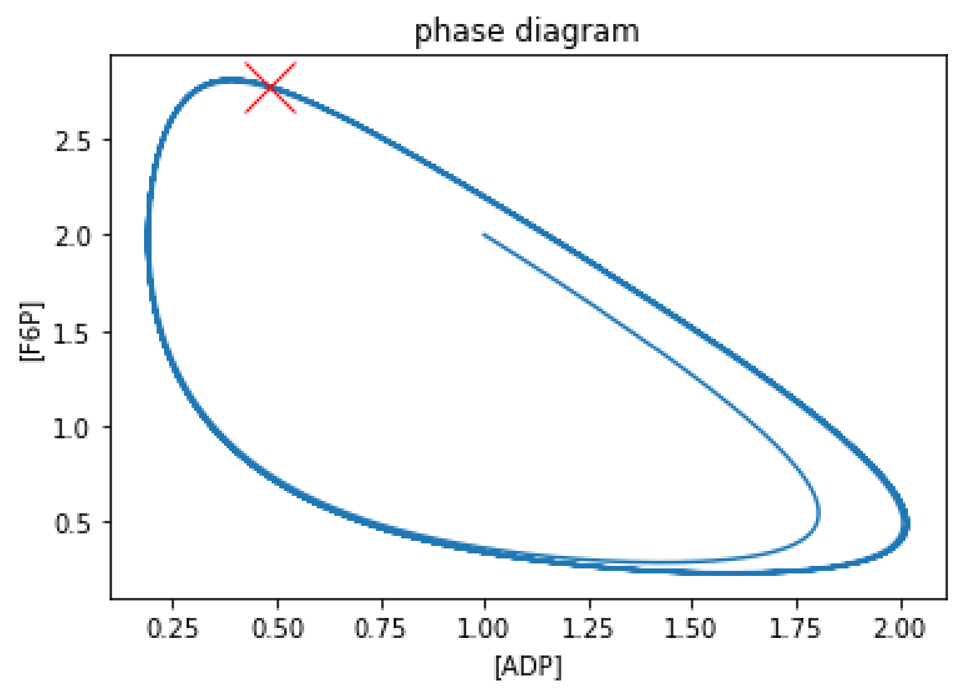
2D system

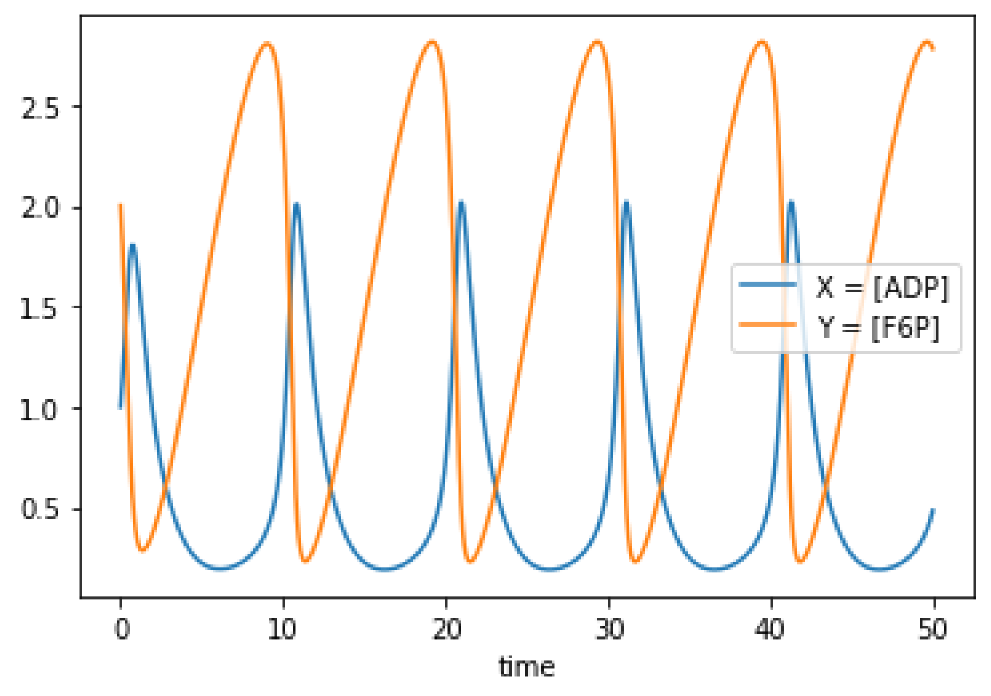


$$P\left(b, \frac{b}{a+b^2}\right) = (0.6, 1.42)$$

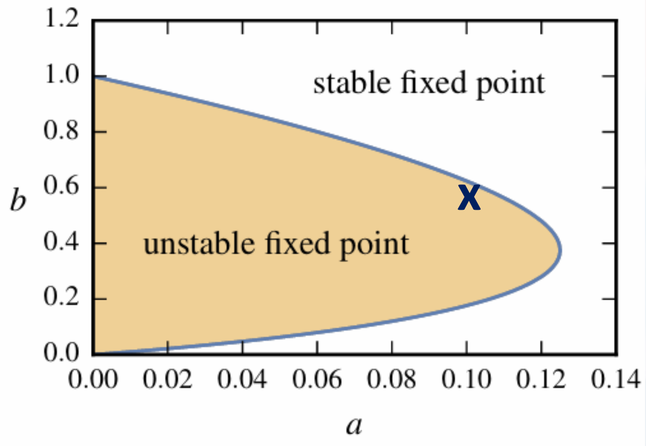
$\dot{x}$ and $\dot{y}$ model **Glycolysis**
(Selkov et al., 1968)

X = [ADP], Y = [F6P]





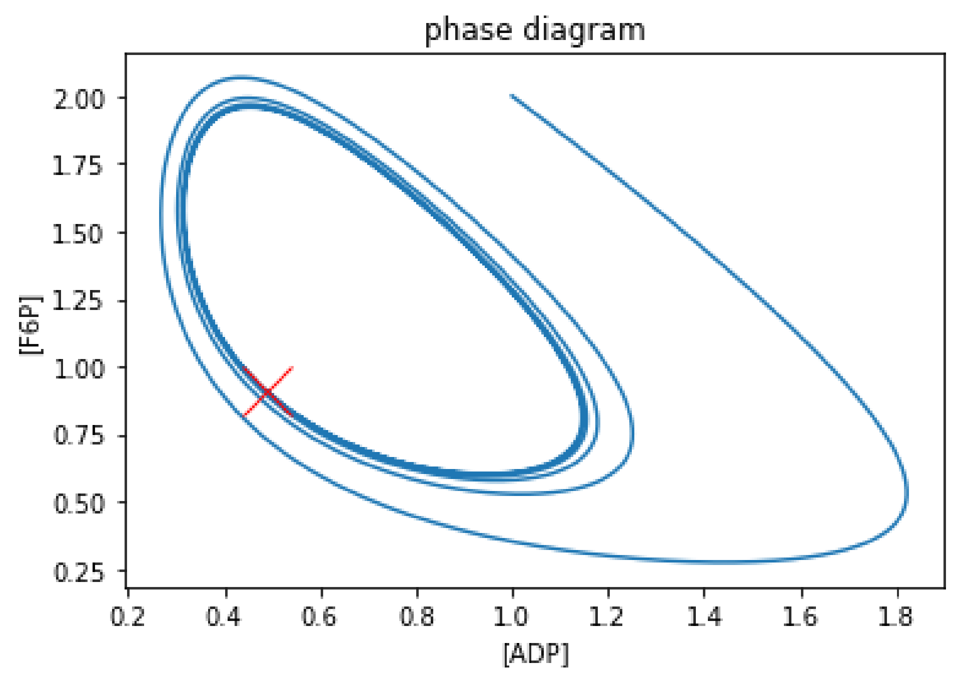
2D system

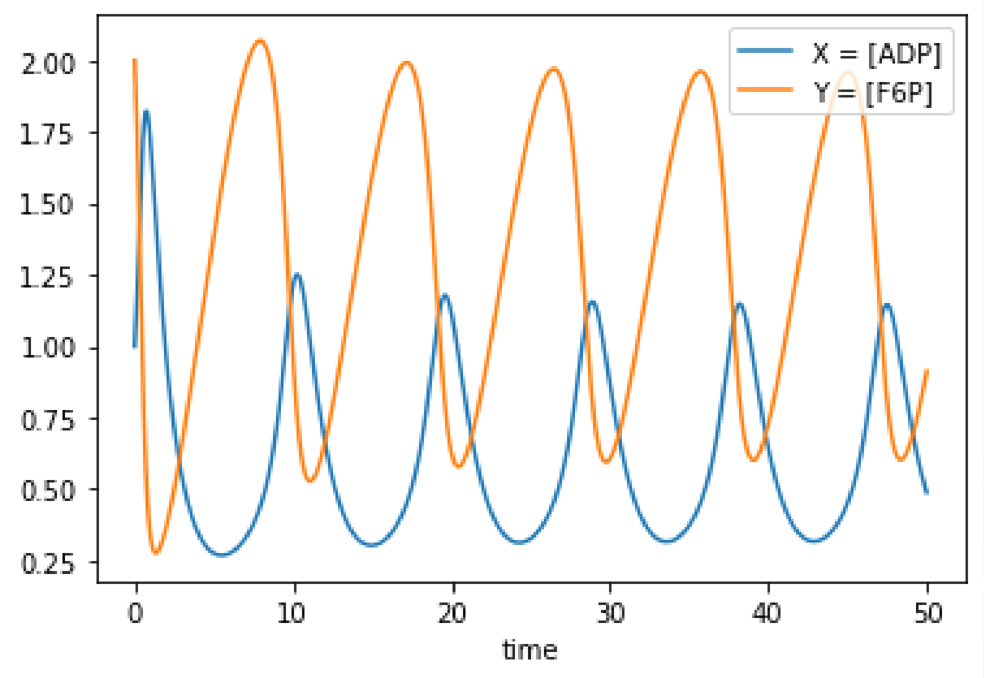


$$P\left(b, \frac{b}{a+b^2}\right) = (0.6, 1.30)$$

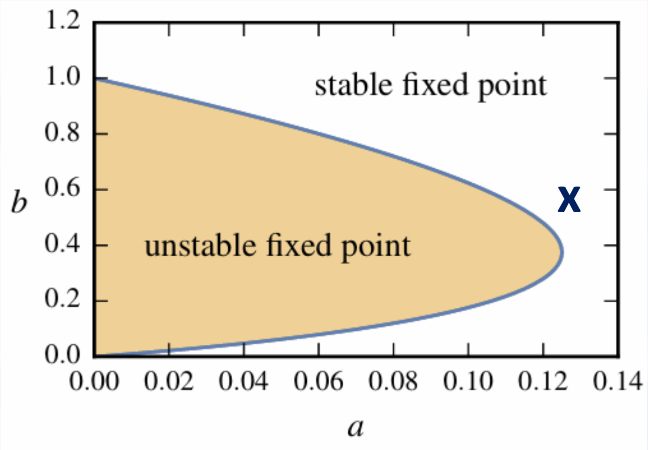
$\dot{x}$ and $\dot{y}$ model **Glycolysis**
(Selkov et al., 1968)

X = [ADP], Y = [F6P]





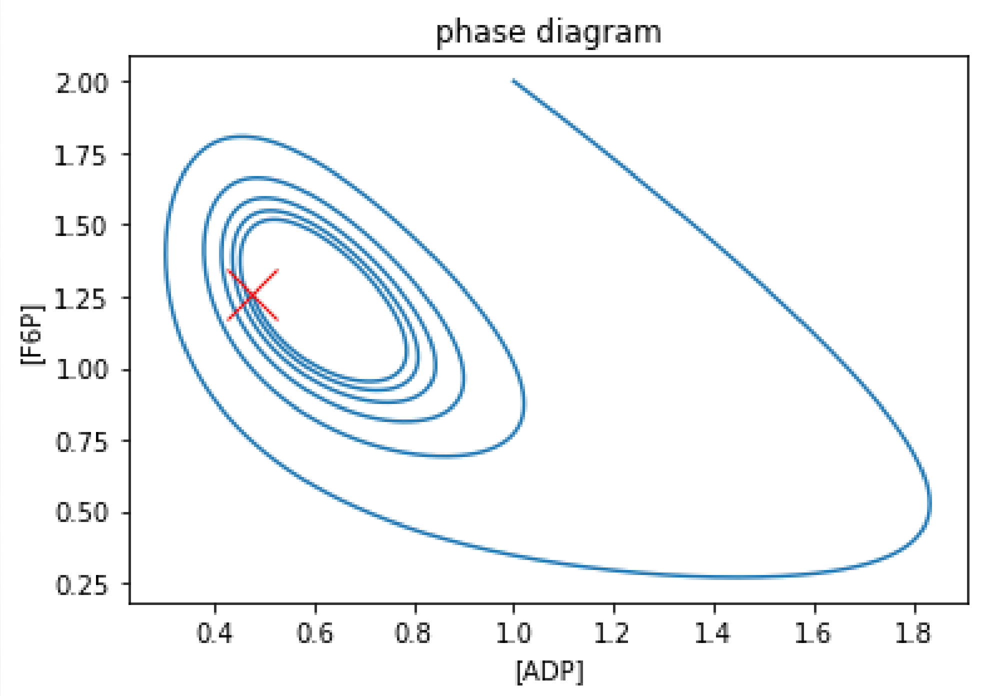
2D system

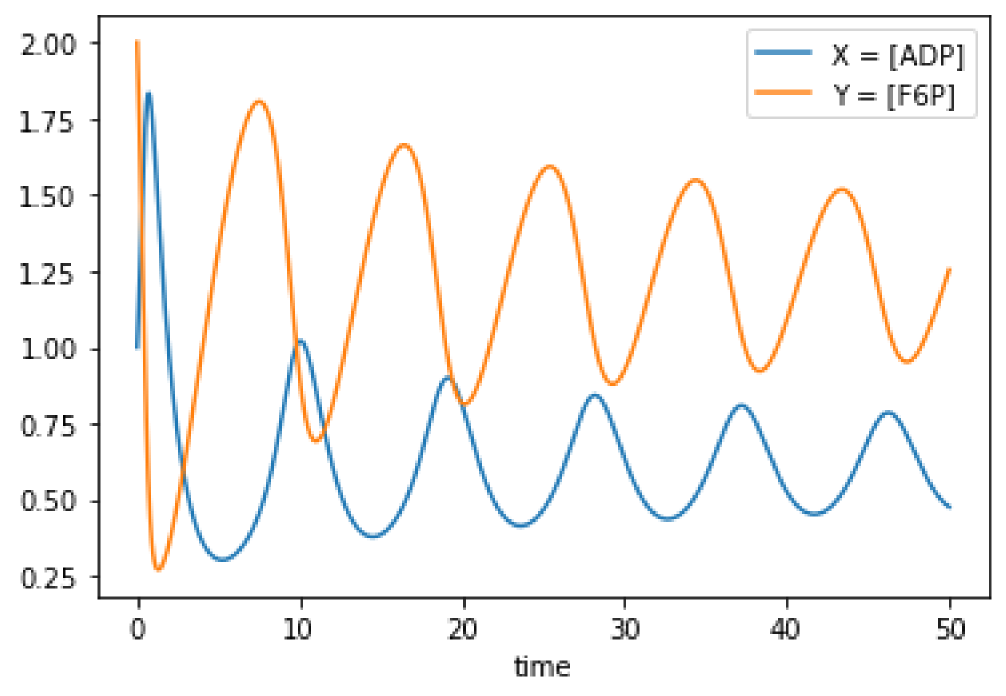


$$P\left(b, \frac{b}{a+b^2}\right) = (0.6, 1.24)$$

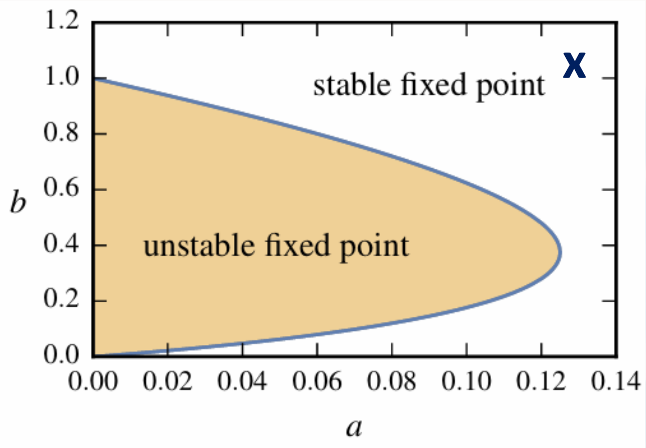
$\dot{x}$ and $\dot{y}$ model **Glycolysis**
(Selkov et al., 1968)

X = [ADP], Y = [F6P]





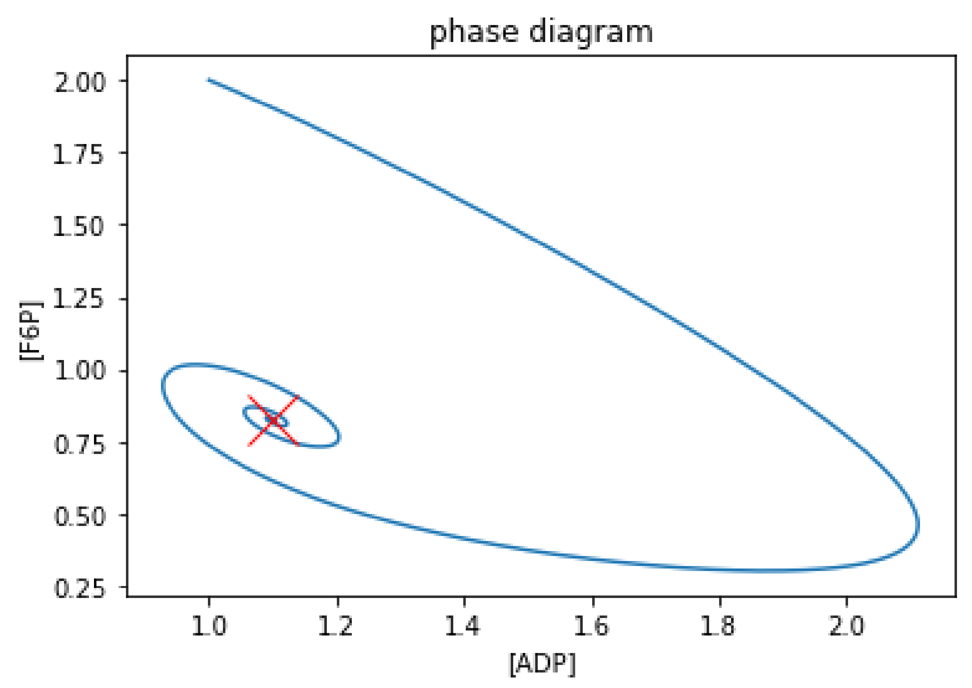
2D system

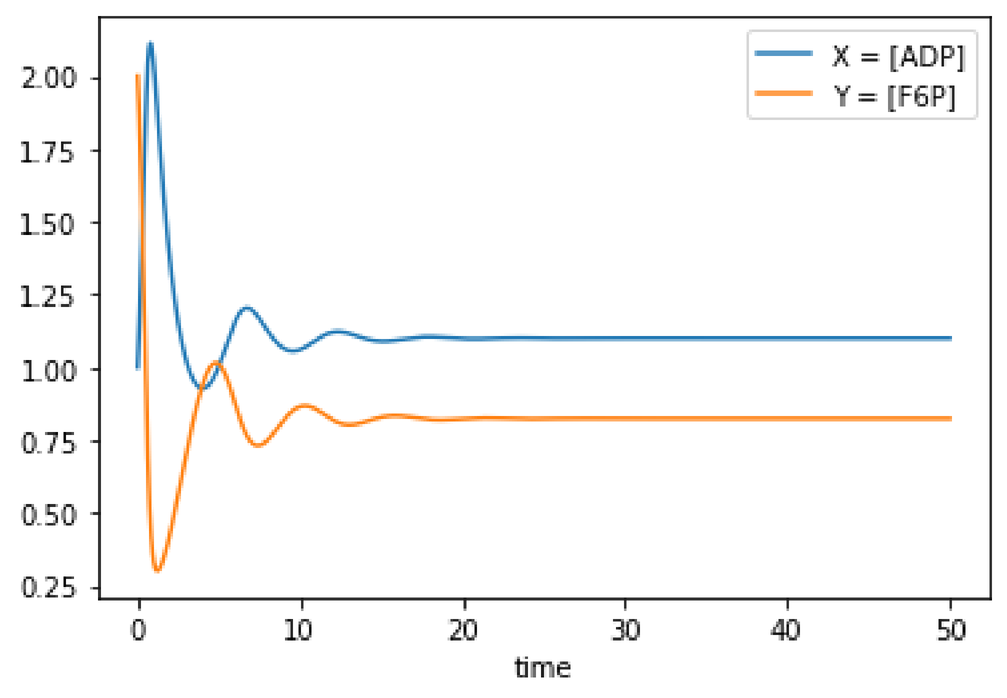


$$P\left(b, \frac{b}{a+b^2}\right) = (1.1, 0.82)$$

$\dot{x}$ and $\dot{y}$ model **Glycolysis**
(Selkov et al., 1968)

X = [ADP], Y = [F6P]





Runge-Kutta-Heun

$\frac{dy}{dt} = f(x(t), t)$ initial condition: $y_0 = y(t_0)$ goal: $y(t)$

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

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

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

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

Runge-Kutta-Heun

$$\frac{dy}{dx_-} = f(x(t), y(x(t)))$$

$$\frac{dy}{dx_+} = f(x(t) + \Delta x, y + \Delta x\, f(x(t)))$$

$$\frac{dy}{dx} = \frac{1}{2}\left[\frac{dy}{dx_-} + \frac{dy}{dx_+}\right]$$

updating:

$$x(new) = x(t) + \Delta x$$

$$y(new) = y(t) + \Delta x \frac{1}{2}\left[\frac{dy}{dx_-} + \frac{dy}{dx_+}\right] = y(t) + \Delta x \frac{1}{2}[f(x(t), y(x(t))) + f(x(t) + \Delta x, y + \Delta x\, f(x(t)))]$$

Runge-Kutta-Heun

$$x(new) = x(t) + \Delta x$$

$$y(new) = y(t) + \Delta x \frac{1}{2}\left[\frac{dy}{dx_-} + \frac{dy}{dx_+}\right] = y(t) + \Delta x \frac{1}{2}[f(x(t), y(x(t))) + f(x(t) + \Delta x, y + \Delta x\, f(x(t)))]$$

more precise (here shown for for 1D *y = y(t)):*

$$k_1 = f(t_n, y_n)$$

$$k_2 = f(t_n + \frac{\Delta t}{2}, y_n + \frac{\Delta t k_1}{2})$$

$$k_3 = f(t_n + \frac{\Delta t}{2}, y_n + \frac{\Delta t k_2}{2})$$

$$k_4 = f(t_n + \Delta t, y_n + \Delta t k_3)$$

$$t(new) = t_{n+1} = t_n + \Delta t$$

$$\mathrm{y}(new) = y_{n+1} = y_n + \frac{\Delta t}{6}\underbrace{[k_1 + 2k_2 + 2k_3 + k_4]}_{\text{recall: Simpson \& Simpson 3/8}}$$

Runge-Kutta-Heun

$$x(new) = x(t) + \Delta x$$

$$y(new) = y(t) + \Delta x \frac{1}{2}\left[\frac{dy}{dx_-} + \frac{dy}{dx_+}\right] = y(t) + \Delta x \frac{1}{2}[f(x(t), y(x(t))) + f(x(t) + \Delta x, y + \Delta x\, f(x(t)))]$$

```
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

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

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

$\dot{x}$ and $\dot{y}$ model **Glycolysis**
(Selkov et al., 1968)

initial values: x(t=0) and y(t=0)

[t_start, t_end]

parameter of the function

contains the actual ODEs

```
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############################

    #...
```

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

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

```
def SolveGlycolysis(Init, t_span, a, b):

    XY      = ode_solver(Glycolysis, Init, t_span, method = 'RK45',\
                        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

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

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

the actual solver

```
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################################

    #...
```

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

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

```python
def SolveGlycolysis(Init, t_span, a, b):

    XY      = ode_solver(Glycolysis, Init, t_span, method = 'RK45',\
                         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),\
                           t_span = t_span, y0 = Init, method = method,\
                           rtol = 1e-9, atol = 1e-9, max_step = 0.01)


        return result
```

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

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

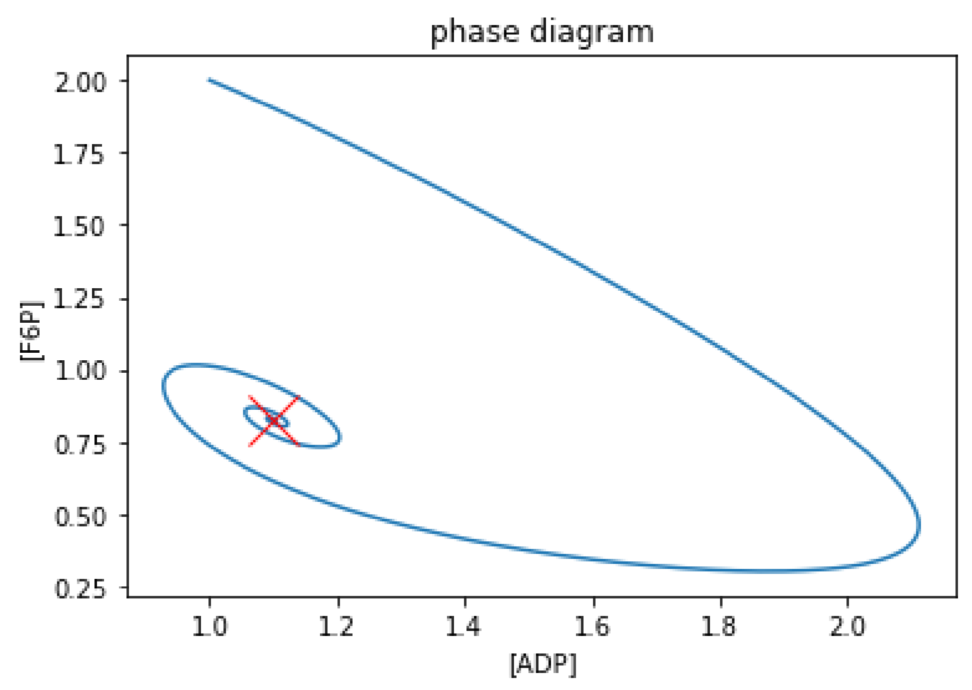
```
def SolveGlycolysis(Init, t_span, a, b):

    XY      = ode_solver(Glycolysis, Init, t_span, method = 'RK45',\
                         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),\
                           t_span = t_span, y0 = Init, method = method,\
                           rtol = 1e-9, atol = 1e-9, max_step = 0.01)


        return result
```

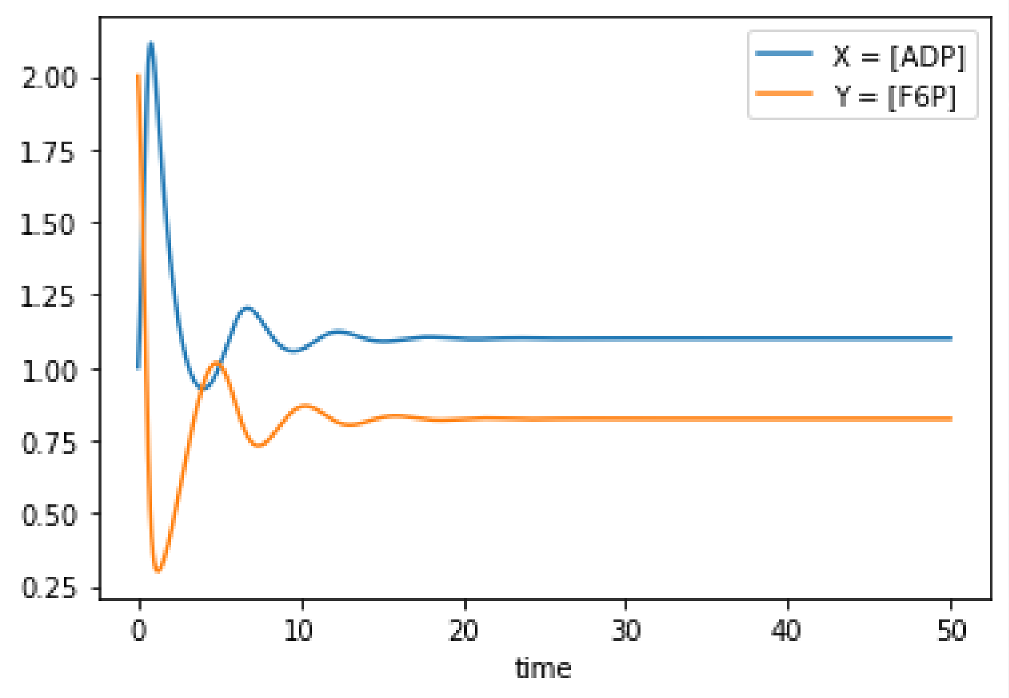
$$\dot{x} = -x + a\,y + x^2 y$$

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

run:

```
a = 0.125
b = 1.1
SolveGlycolysis([1, 2], [0, 50], a, b)
```





run:

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

Synergistic elimination of bacteria by phage and the immune system

Chung Yin (Joey) Leung* and Joshua S. Weitz†
School of Biology, Georgia Institute of Technology, Atlanta, Georgia 30332, USA and
School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332, USA

$$\dot{B} = \boxed{\overbrace{rB\left(1-\frac{B}{K_C}\right)}^{\text{Growth}}} - \overbrace{\phi BP}^{\text{Lysis}} - \overbrace{\frac{\epsilon IB}{1+B/K_D}}^{\text{Immune killing}},$$

$$\dot{P} = \overbrace{\beta\phi BP}^{\text{Replication}} - \overbrace{\omega P}^{\text{Decay}},$$

$$\dot{I} = \overbrace{\boxed{\alpha I\left(1-\frac{I}{K_I}\right)}\frac{B}{B+K_N}}^{\text{Immune stimulation}}.$$

B:	bacteria
P:	phages
I:	immune cells

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

recall:
Verhulst Equation

<u>run:</u>

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

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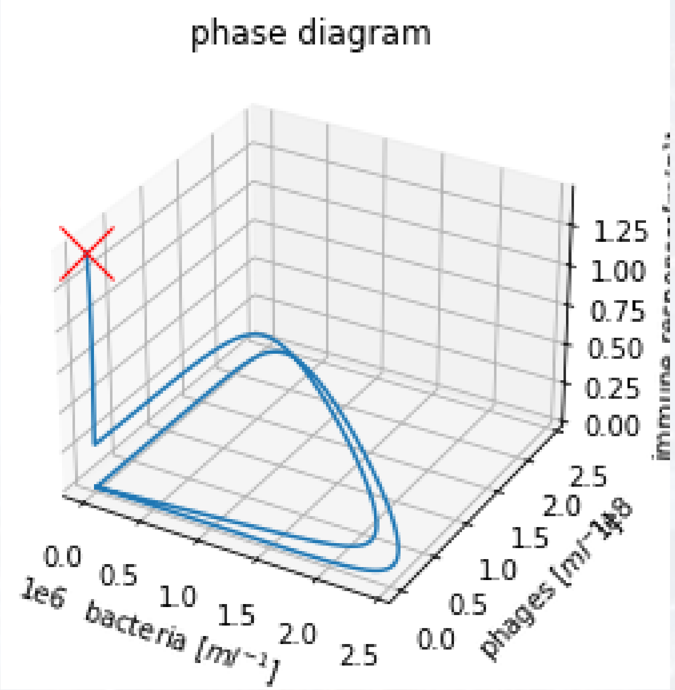

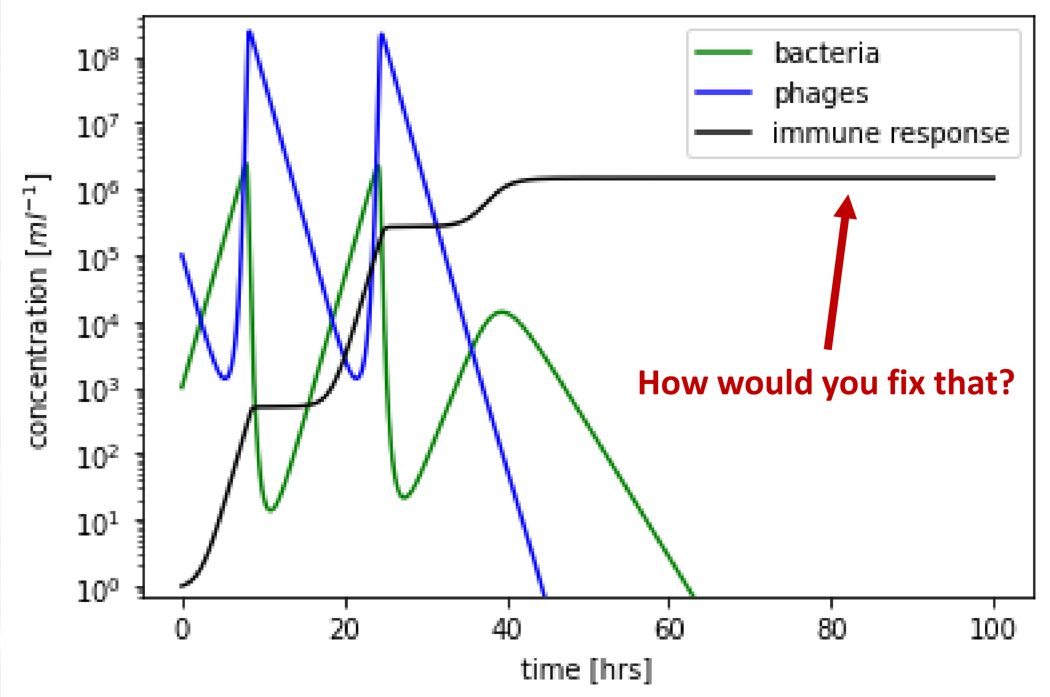

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Thank you for your attention!