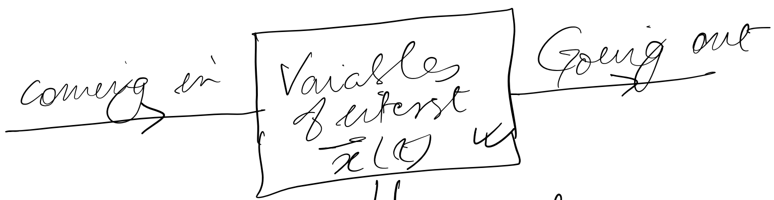
Sept 11, 2024

Chapter 2: Modeling with Ordinary Differential Equations (ODEs).

☒ Modeling through initial value problems.

t: independent variable (time)

$\vec{x}(t)$: $(x_1(t), x_2(t), \dots, x_n(t))$: Variables of interest as a function of time.



$\Downarrow$ Model

Differential Equations: Continuous-time Dynamical System.

Rate of Change = Coming in − Going out

$$\frac{d\vec{x}(t)}{dt} = \underbrace{\text{Coming in} - \text{Going out}}_{u}$$

$$\boxed{\frac{d\vec{x}}{dt} = \vec{f}(\vec{x}, \vec{p})}$$

- $\vec{p} = (p_1, p_2, \dots, p_k)$ parameters.

$$\Longleftrightarrow \begin{cases} \dfrac{dx_1(t)}{dt} = f_1(\vec{x}, \vec{p}) \\ \dfrac{dx_2(t)}{dt} = f_2(\vec{x}, \vec{p}) \\ \vdots \\ \dfrac{dx_n(t)}{dt} = f_n(\vec{x}, \vec{p}) \end{cases}$$

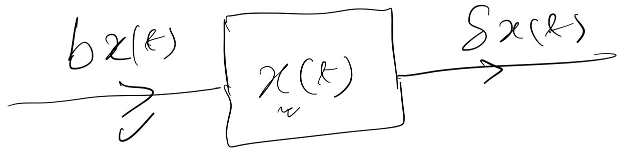
Example:

1. Single variable (species) model with birth-death process:

$x(t)$: Quantity (population) at time t.

b: birth rate per individual (per capita)

δ: death rate per individual (per capita)



Rate of change of population = IN − OUT

$$\frac{dx}{dt} = bx(t) - \delta x(t)$$

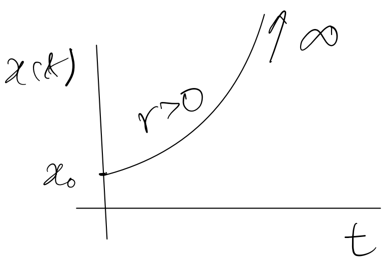
$$\Rightarrow \frac{dx}{dt} = (b-\delta)x(t)$$

$$\Rightarrow \boxed{\frac{dx}{dt} = r x(t)},$$

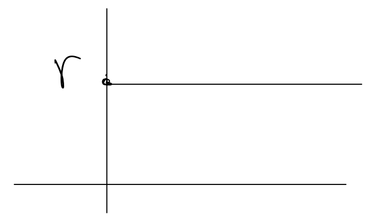
$r = b - \delta$, per capita growth rate.

(In case of population, this is Malthusian growth.)

Limitation:



Because



2. Single species logistic model

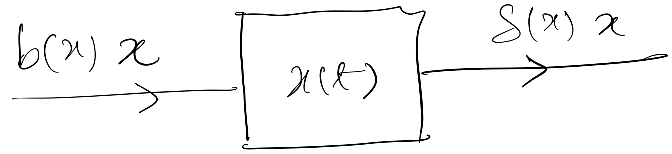
$b(x)$: birth rate
$\delta(x)$: death rate
} because of competition due to resource constraints

$\Downarrow$

$b(x) \downarrow$

$\delta(x) \uparrow$

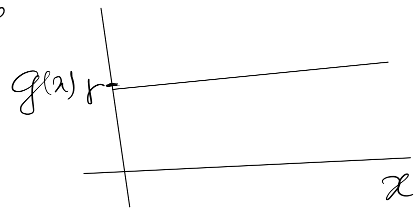
$\Downarrow$ $g(x) = b(x) - \delta(x)$



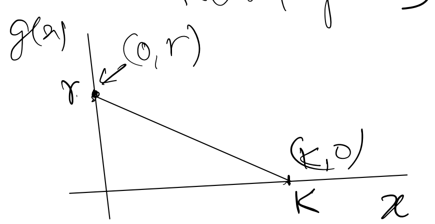
$$\frac{dx}{dt} = \left(b(x) - \delta(x) \right) x$$

$$\frac{dx}{dt} = g(x)\, x$$

Previous



New (logistic)



$$g(x) = \frac{0-r}{K-0}\, x + r$$

$$= r\left(1 - \frac{x}{K}\right)$$

$$\therefore \boxed{\frac{dx}{dt} = r x \left(1 - \frac{x}{K}\right)}$$

Logistic Model.

$$= rx - \frac{r}{K} x^2$$

→ self regulating or self limiting due to competition of resources.

growth if $x << K$

i.e; $\frac{x}{K} << 1$

i.e $\frac{r}{K} x^2 \simeq 0$

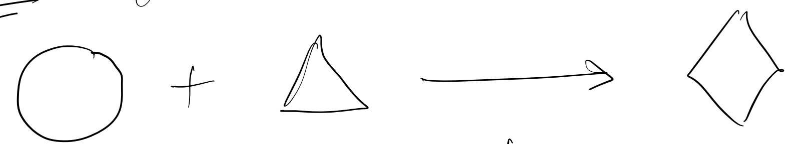
3. Chemical (Biochemical reaction).

- Biochemical kinetics concerns the concentration of chemical substances in biological systems as function of time.
- Biochemical kinetics are often controlled by enzyme catalysts (that are present in low

concentration, but have a large effect on the rate process }.

Law of Mass Action:

The rate of chemical reaction



$$\boxed{A} + \boxed{B} \xrightarrow{k} \boxed{C}$$

is given by kAB, where A and B are concentration of chemicals

k: rate constant

The model for this reaction is (RATE = IN − OUT)

$$\frac{dA}{dt} = -kAB$$

$$\frac{dB}{dt} = -kAB$$

$$\frac{dC}{dt} = kAB$$

If back reaction is considered, i.e.,

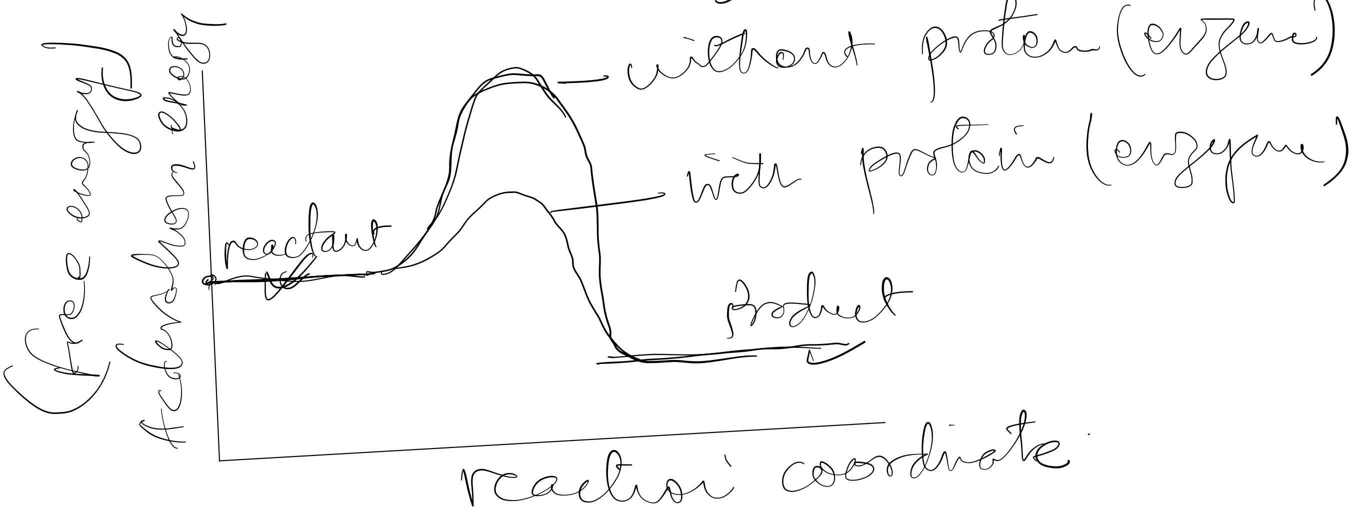
$$\boxed{A} + \boxed{B} \underset{k_-}{\overset{k_f}{\rightleftharpoons}} \boxed{C}$$

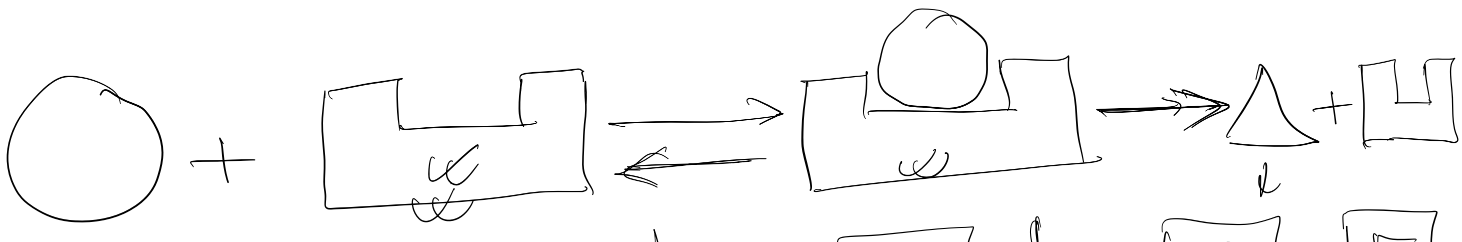
$$\frac{dA}{dt} = -k_f AB + k_- C$$

$$\frac{dB}{dt} = -k_f AB + k_- C$$

$$\frac{dC}{dt} = k_f AB - k_- C.$$

- Reaction catalized by an enzyme (biochemical reaction).





$$S + E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C \xrightarrow{k_2} P + E$$

Model:

$$\begin{cases} \dfrac{dS}{dt} = k_{-1}C - k_1 SE \\ \dfrac{dE}{dt} = k_{-1}C + k_2 C - k_1 SE \\ \dfrac{dC}{dt} = k_1 SE - k_{-1}C - k_2 C \\ \dfrac{dP}{dt} = k_2 C \end{cases}$$

$$\frac{d}{dt}(E+C) = \frac{dE}{dt} + \frac{dC}{dt} = k_{-1}C + k_2C - k_1SE + k_1SE - k_{-1}C - k_2C = 0$$

$\Rightarrow \quad E + C = E_0$, a constant

or $E = E_0 - C$ (total amount of enzyme is conserved)

Also, $\frac{d}{dt}(S + C + P) = 0$

$\Rightarrow \quad S + C + P = S_0$, constant (substrate conserved)

$\therefore$ the system reduces to

$$\left.\begin{aligned} \frac{dS}{dt} &= k_{-1} C - k_1 S (E_0 - C) \\ \frac{dC}{dt} &= k_1 S (E_0 - C) - (k_{-1} + k_2) C \end{aligned}\right\}$$

$E = E_0 - C, \quad P = S_0 - S - C.$