BS - 3COMATH1 - S1 - Modeling biological dynamics with ordinary differential equations

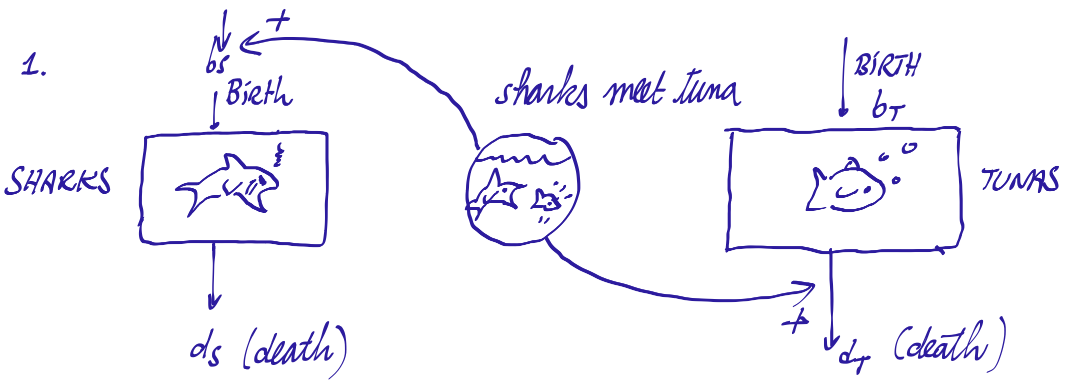
Introduction to modeling skills 1/2

Exercise 1

S: number of sharks $\quad S(t) \quad S(0) = S_0 > 0$

T: " of tunas $\quad T(t) \quad T(0) = T_0 > 0$

1.

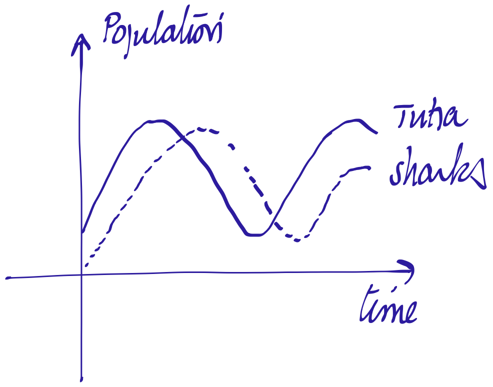


2. $S'(t) = b_S\, S(t) - d_S\, S(t) + k\beta\, S(t)\, T(t)$

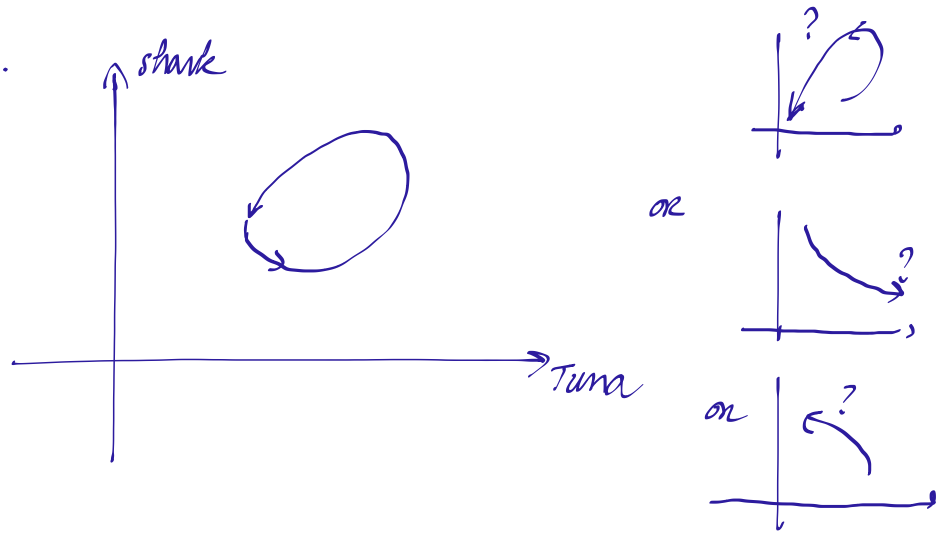
$T'(t) = b_T\, T(t) - d_T\, T(t) - \beta\, S(t)\, T(t)$

$\alpha_T T(t) - \beta S(t) T(t)$

3.



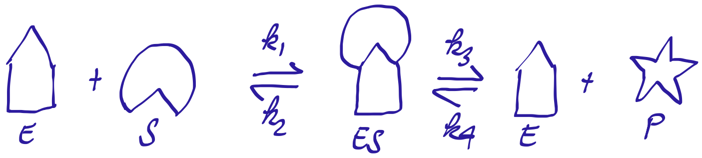
4.



5. Cycle, a co-existence or death of sharks or death of both populations

Exercise 2 Michaelis-Menten equations

1



$$E + S \underset{k_2}{\overset{k_1}{\rightleftharpoons}} ES \underset{k_4}{\overset{k_3}{\rightleftharpoons}} E + P$$

2 i) product formation is not reversible $\Rightarrow$ $\boxed{k_4 = 0}$

ii) binding of E and S is much faster than the release of P

k_1 and $k_2 \gg k_3$

k_1 and $k_2 \gg k_3$

Thus, $\frac{d[ES]}{dt} = 0$ (steady state)

$$E + S \underset{k_2}{\overset{k_1}{\rightleftharpoons}} ES \xrightarrow{k_3} E + P$$

③ a. $E + S \xrightarrow{k_1} ES$

$v_f = k_1 [E][S]$ law of mass action

b. $E + S \xleftarrow[k_2]{} ES \xrightarrow[k_3]{} E + P$

$v_e = (k_2 + k_3)\, ES$

c. $\frac{d[ES]}{dt} = v_f - v_e = k_1 [E][S] - (k_2 + k_3)[ES]$

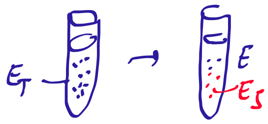
d. $\frac{d[ES]}{dt} = 0 \Leftrightarrow v_f = v_e$. Thus $k_1 [E][S] = (k_2 + k_3)[ES]$

$\Rightarrow [E][S] = \frac{k_2 + k_3}{k_1}[ES] = K_M [ES]$

Michaelis constant

e. $[E][S] = K_M [ES]$

④ a. $[E_T] = [E] + [ES]$



b. Since $[E][S] = K_M [ES]$ and $[E] = [E_T] - [ES]$

Then $([E_T] - [ES])[S] = K_M [ES]$

$\Leftrightarrow [E_T][S] - [ES][S] = K_M [ES]$

$\Leftrightarrow [E_T][S] = [ES](K_M + [S])$

$\Leftrightarrow [ES] = \frac{[E_T][S]}{}$

$\Leftrightarrow \quad [ES] = \dfrac{[E_T][S]}{K_M+[S]}$

$ES \xrightarrow{k_3} E+P$

c. we know that $\dfrac{dP}{dt} = k_3 [ES]$

b. $\quad = k_3 \dfrac{[E_T][S]}{K_M+[S]}$

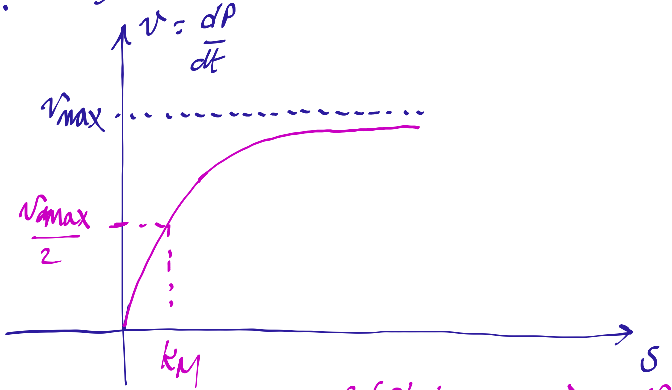
If we note $v = \dfrac{dP}{dt}$ $\quad v = \dfrac{k_3 [E_T][S]}{K_M+[S]}$

d. when $[S] \to +\infty$ $\quad v \to k_3[E_T]$ denote $v_{max} = k_3[E_T]$

then $\boxed{v = v_{max} \dfrac{[S]}{K_M+[S]}}$: equation of Michaelis

5.

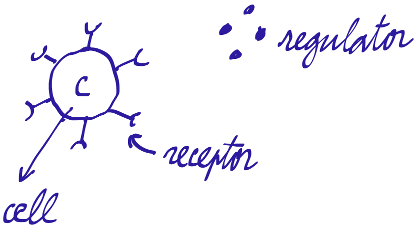
6.

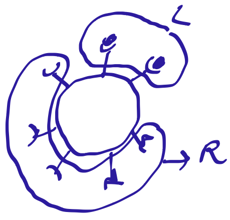


If $[S] = K_m$ $\quad v = v_{max}/2$

Exercise 3: Hill function

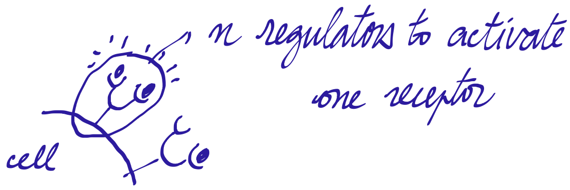
1.





$[R] + [L] = m[C]$

- n regulators to activate



2. $R + nG \overset{K}{\rightarrow} L \quad \Rightarrow \quad [R][G]^n = K[L]$

3. a. $F = a \dfrac{[L]}{m[C]}$

b. $[R][G]^n = K[L] \Rightarrow [L] = \dfrac{[R][G]^n}{K}$

and $[R] + [L] = m[C]$

so $[L] = \dfrac{(m[C] - [L])[G]^n}{K}$

$\Leftrightarrow \quad K[L] + [L][G]^n = m[C][G]^n$

$\Leftrightarrow \quad [L]\left(K + [G]^n\right) = m[C][G]^n$

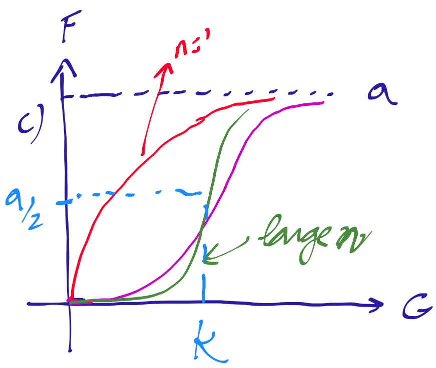
$\Leftrightarrow \quad [L] = \dfrac{m[C][G]^n}{K + [G]^n}$

$\Leftrightarrow \quad \dfrac{[L]}{m[C]} = \dfrac{[G]^n}{K + [G]^n}$

$\Leftrightarrow \quad \overset{''}{F/a} = \dfrac{[G]^n}{K + [G]^n}$

$\Leftrightarrow \quad F = a \dfrac{[G]^n}{K + [G]^n}$

c)



$K =$

If $[G] = k$ $\quad F = \frac{ak}{k+k} = \frac{a}{2}$

d. If $n \to +\infty$: denote $f : x \mapsto \frac{ax^n}{k+x^n}$

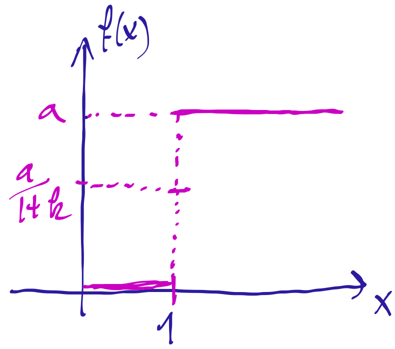
$$f(x) = \frac{ax^n}{k+x^n} = \frac{ae^{n\ln x}}{k+e^{n\ln x}}$$

if $0 < x < 1$: $\ln x < 0$ $\quad e^{n\ln x} \xrightarrow[n\to+\infty]{} 0$ $\quad f(x) = 0$

if $x = 1$ $\quad n\ln 1 = 0$ $\quad e^{n\ln x} = 1$ $\quad f(x) = \frac{a}{1+k}$

if $x > 1$ $\quad n\ln x > 0$ $\quad e^{n\ln x} \to +\infty$ $\quad \frac{\cancel{e^{n\ln x}}}{\cancel{e^{n\ln x}}}\left(\frac{a}{\frac{k}{e^{n\ln x}}+1}\right) \longrightarrow \frac{a}{0+1} = a$

"$n = +\infty$"



case $n = +\infty$
"bang-bang" kinetics