1st application of GIBBS FREE Energy → Phase equilibrium.

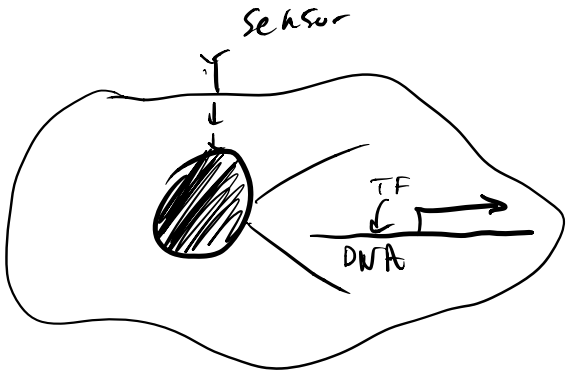
2nd → Chemical Reaction Equilibrium + Calculations

Focus now on cell signaling, gene control, reactions, & what's Gibbs got to do with it?

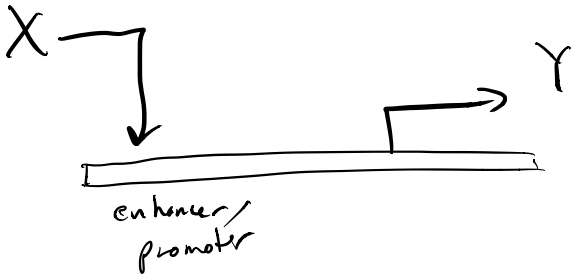
Gene activation
- Logic model
- Hill functions
- on/off kinetics

Gene repression
- Logic models
- Hill functions
- on/off kinetics.

Differential mass balance equations.



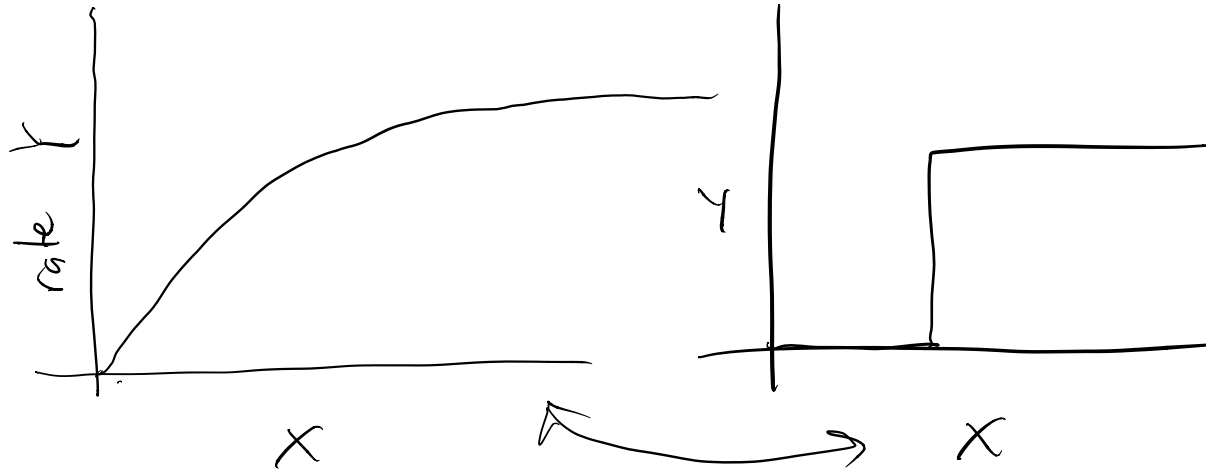
TF: Transcription Factor X
and X activates Y

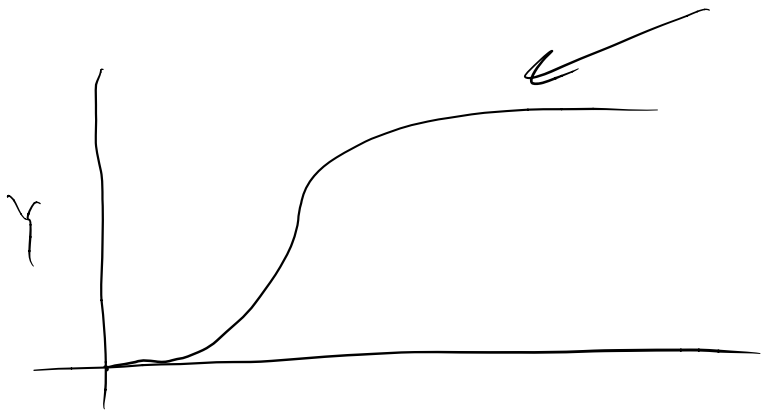


Rate of transcription of Y as a fcn of X?

$$\text{rate} = \frac{dY}{dt} = f(X)$$

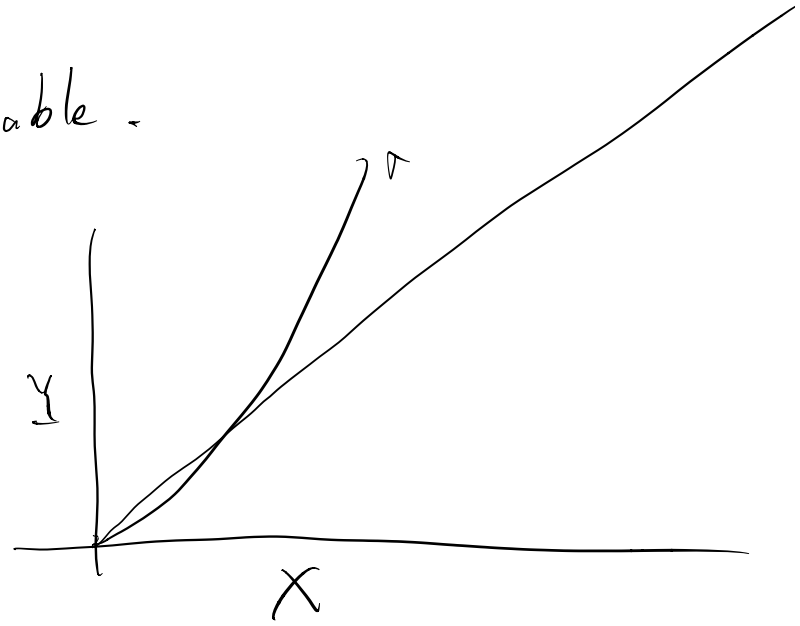
What relationship / function makes sense?

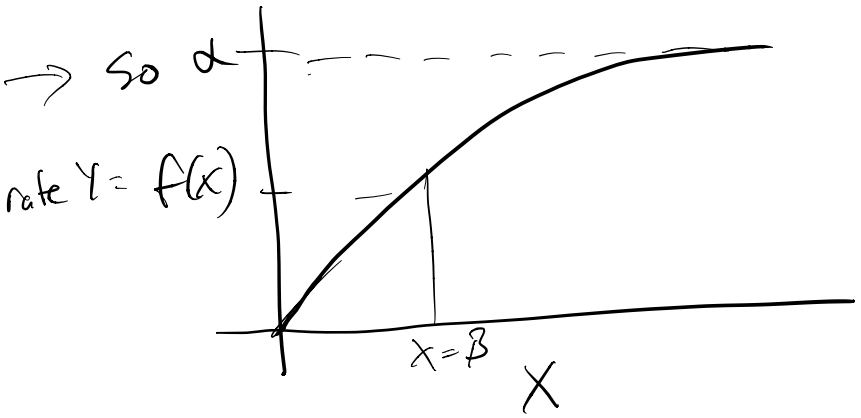




All reasonable.

Unreasonable

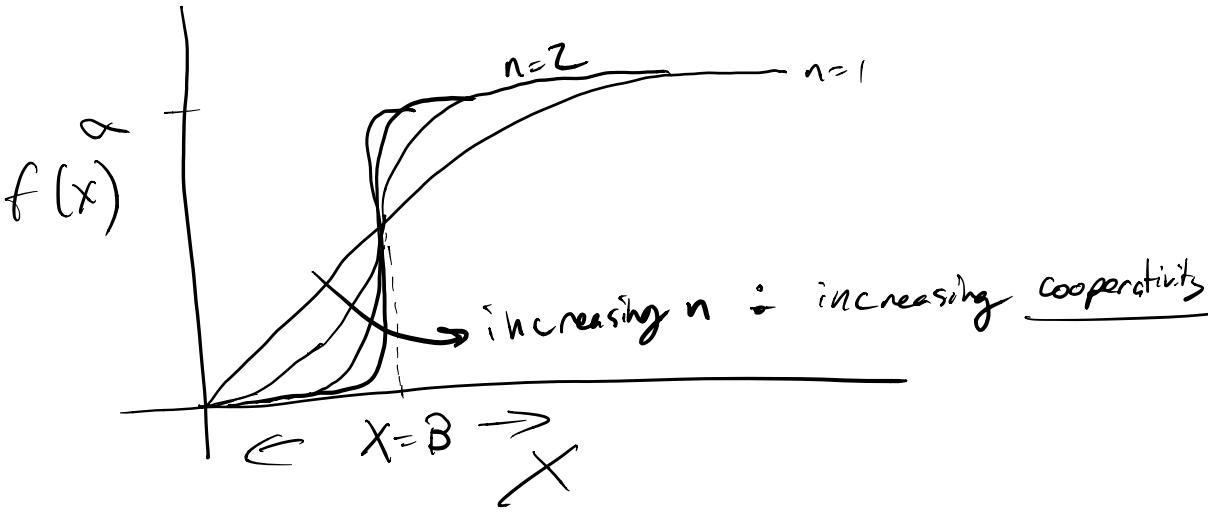




$f(x) = \dfrac{\alpha X}{\beta + X}$

↙ Saturation equation

$$f(x) = \frac{\alpha X^n}{\beta^n + X^n}$$



β determines the position of the switch in slope (left or right)

Hill functions

parameters $f(X) = \frac{\alpha X^h}{B^n + X^n}$

α: maximum possible expression rate

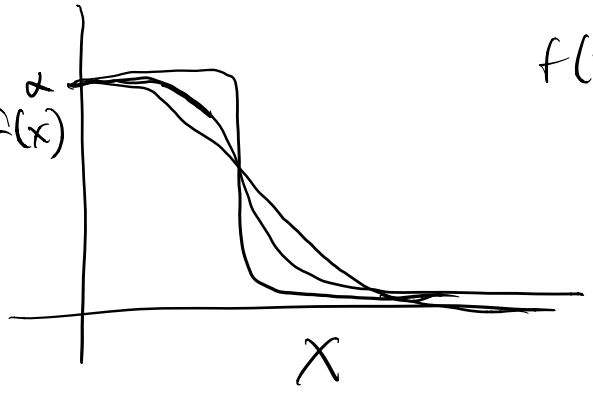
B: the effective concentrations of X

B is equal to the concentration of X when at half-max gene expression

---

Repression:

rate $Y = f(x)$



$f(x) = \frac{\alpha}{1 + \left(\frac{X}{B}\right)^n}$

Two simple functions

Making the equations

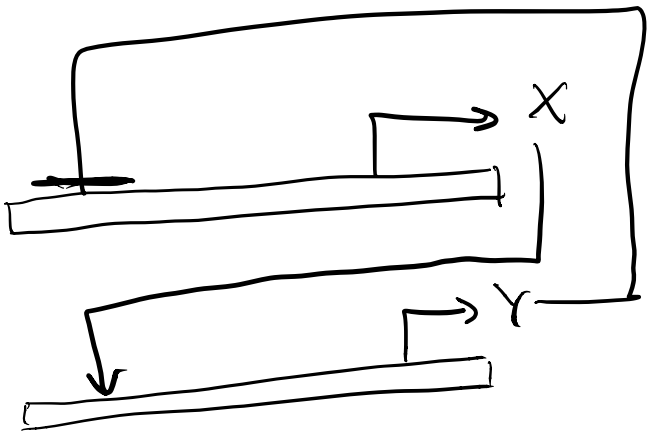
1) Everything decays - or has a lifetime.

Differential equation for activation of Y for some X.

$$\frac{dY}{dt} = \frac{\alpha_1 X^n}{\beta_1^n + X^n} - \kappa \cdot Y$$

Accumulation — Generation — Consumption

model for concentration of Y in cell as a function of X and time.



- make the equations for X, Y

$$\frac{dX}{dt} = \frac{\alpha_1}{1 + \frac{Y^n}{\beta_1^n}} - k_1 \cdot X$$

$$\frac{dY}{dt} = \frac{\alpha_2 X^n}{\beta^n + X^n} - k_2 \cdot Y$$

Next time, we will start to solve the differential equations in Matlab.