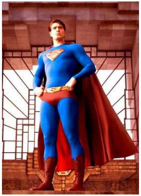
Outline

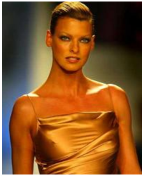
- Modeling intro
- First order chemical kinetics.
- Second order chemical kinetics.

Modeling

- A model is an abstract representation of an object, system, or process, usually idealizing some features and neglecting others.



For a population with heritable variation in some characteristic that inuences an individual's capacity to reproduce or success in reproduction, the frequency of those phenoptypes that reproduce most successfully will increase.



$$\frac{\partial u}{\partial t} = D\nabla^2 u$$

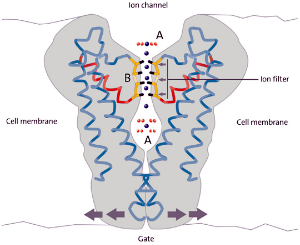
Modeling and theories

- Mathematical models are one category of *theory*, consisting of a set of assumptions (axioms), an agreed upon language (mathematics), and a framework of acceptable means of drawing conclusions from the axioms (logic).
- Mathematical models are formulated through translating real phenomena into parameters, variables and their interrelations which often come in the form of differential equations.
- Example: Assume that the size of a population of bacteria grows at a rate proportional to its current size (our assumption). Translating into an equation, we get $dp/dt = rp$ (the assumption restated in our mathematical language). Solving this equation (an acceptable means of drawing conclusions), we find that the population grows exponentially. To determine if we've got a good theory, we must look at data.

Chemical kinetics

First order kinetics

- A reaction whose rate depends on the concentration of only one reactant.
- Example: an ion channel undergoing a conformation change (closed to open).

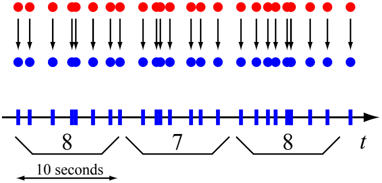


(From `http://www.bio.miami.edu/~cmallery/150/memb/ion_channels.htm`)

Chemical kinetics

First order kinetics

- When is it reasonable to claim that for a collection of 100 molecules, we can determine the average rate of the reaction?



Estimate of reaction rate: $\lambda = 7.7$ reactions per 10 seconds per 100 molecules $= 0.077\ \mathrm{s}^{-1}\ \mathrm{molecule}^{-1}$

Chemical kinetics

First order kinetics

- $N(t)$ unreacted molecules at time t. Change in $N(t)$:

$$N(t + \Delta t) = N(t) - \lambda \Delta t N(t).$$

$$N(t + \Delta t) - N(t) = -\lambda \Delta t N(t).$$

$$\frac{N(t + \Delta t) - N(t)}{\Delta t} = -\lambda N(t).$$

Chemical kinetics

First order kinetics

$$\frac{N(t+\Delta t) - N(t)}{\Delta t} = -\lambda N(t).$$

- In the limit $\Delta t \to 0$,

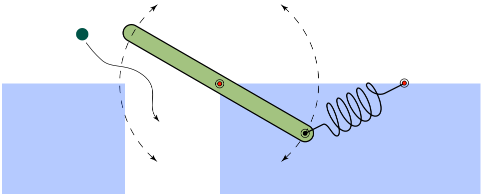
  $$\frac{dN}{dt} = -\lambda N.$$

  Valid only for periods of time long enough for the average rate to give a good approximation of the number of reactions. More molecules $\Rightarrow$ short time intervals are ok.
- What determines λ, the average rate?

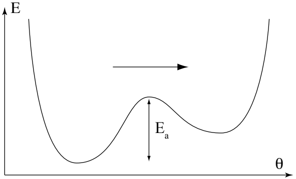
Chemical kinetics

First order kinetics

- Full protein structure too hard to analyze; build a simpler model...



- Energy as a function of gate angle:

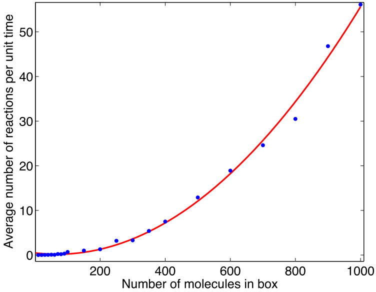


- Average rate $\propto e^{-E_a/kT}$. Matlab movies...

Chemical kinetics

Second order kinetics

- Reaction of two molecules, possibly of the same type, requiring a collision.
- Harder to describe because of space, diffusion and collision.
- Take N molecules, place in box, let them diffuse. If two collide, give them a prob p of reacting. How does the rate scale with N? More movies...



- The reaction rate equation:

$$\frac{dN}{dt} = -kN^2.$$