BCB 570

Class info

- Tasos (Anastasios) Matzavinos: tasos@iastate.edu
- Formal office hours after class, 4-5pm MWF (informally by appointment)
- Grading scheme: 40% homeworks, 60% class projects

Class organization

0.0.1 Kinetic modeling of metabolic networks

- deterministic and stochastic models
- structural analysis of networks
- extreme pathways
- flux cones
- XPP software

0.0.2 Analysis of high-throughput (genomic) data

- clustering
- kernelized SVMs

0.0.3 Transcription networks

- motifs
- random graphs
- scale-free networks
- regulatory networks

Kinetic modeling: the dynamics of simple decay

Consider the reaction

$$M \rightarrow \emptyset$$

in which molecules of substance M degrade into some substance we are not interested in tracking. Let the function $M(t)$ represent the number of molecules of M at time t. Now, assume that every minute, 2 out of every 100 molecules of M degrade. Thus, the *probability* p_1 of a molecule degrading within the time span of a minute is $\frac{2}{100} = \frac{1}{50} = 0.02 = p_1$. The *rate* k_1 of the reaction is the probability per unit time: in this case, $k_1 = \frac{1}{50}$ molecules per minute.

Let p_n be the probability of degredation within n minutes.

$$p_2 = \frac{2}{100} + \frac{2}{100} = \frac{4}{100} = \frac{1}{25}$$

$$k_2 = \frac{p_2}{2} = \frac{\frac{1}{25}}{2} = \frac{1}{50} = k_1$$

Therefore, while the probability of degredation depends on time, the reaction rate does not. We can write this reaction as a *discrete time model*.

$$M(t + \Delta t) = M(t) - p_{\Delta t} M(t)$$

$$M(t + \Delta t) - M(t) = -p_{\Delta t} M(t)$$

$$\frac{M(t + \Delta t) - M(t)}{\Delta t} = \frac{-p_{\Delta t}}{\Delta t} M(t) = -kM(t)$$

If we let $\Delta t \to 0$, we have the differential equation

$$\frac{d}{dt}M(t) = -kM(t)$$

with solution

$$M(t) = M(0)e^{-kt}$$

Law of mass action

This law is only applicable when molecular species are present in an abundance. It is also only applicable to *elementary reactions* (to be defined).

Consider a reaction

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

in which the rate k refers to the accumulation of molecule C. We are interested in calculating the concentration of C $[C]$. The Law of Mass Action identifies $\frac{d}{dt}[C]$ with the (mathematical) product $k[A][B]$.

Now consider the reversible extension of this reaction.

$$\mathrm{A} + \mathrm{B} \underset{k^-}{\overset{k^+}{\rightleftharpoons}} \mathrm{C}$$

If we want to measure $[A]$, we have the following differential equation.

$$\frac{d}{dt}[A] = k^-[C] - \frac{d}{dt}[C]$$

$$\frac{d}{dt}[A] = k^-[C] - k^+[A][B]$$

We will cover the Law of Mass Action in more detail during the next lecture.