Lecture: Chem 440 #1

Welcome to pchem!

Our goal: quantitative understanding of molecules and chemical reactions from "First Principles"

TAs will make notes available if you have to miss lectures

Course policies: see our website (link in chat)

The math of pchem: ① Averages

e.g. $y_i = 1, 3, 2, 3, 4, 4 \qquad N = 6$

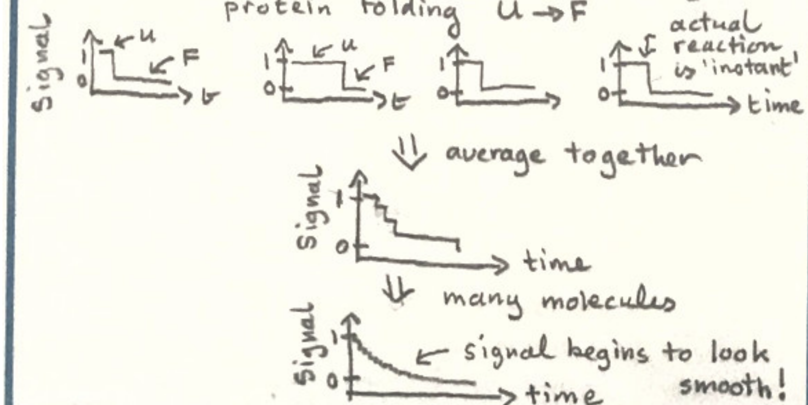
$$\bar{y} = \frac{1+3+2+3+4+4}{6} \approx 2.83$$

$$= \frac{1}{6}\cdot 1 + \frac{2}{6}\cdot 3 + \frac{1}{6}\cdot 2 + \frac{2}{6}\cdot 4 = \sum_i P_i \cdot y_i$$

$\sum P_i =$ ↓ probability; value

If $y_i \to y(x)$, a continuous function, then the sum becomes an integral: $\bar{y} = \int P(x)\cdot y(x)\,dx$

Example: Single molecule reaction, e.g. protein folding $U \to F$

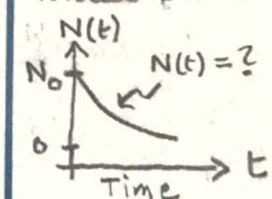


② Derivative models.

e.g. $\frac{\partial x}{\partial t} = f(x, t)$

The irony: chemical systems are discrete molecules, so it is $\frac{\Delta x}{\Delta t}$, and $\frac{\partial x}{\partial t}$ is the approximation!

Example: Start with many ($N_0 \gg 1$) unfolded proteins. How many are left at time t?



Thought: "The rate at which unfolded proteins fold is proportional to the number of unfolded proteins"

Turning the words into an equation:

$$\frac{\partial N}{\partial t} \sim N \quad \text{or} \quad \frac{\partial N}{\partial t} = -\underbrace{k}_{\text{proportionality constant}} N$$

Q: Why the minus sign

Solving, (dummy variables)

$$\frac{dN}{N} = -k\,dt \Rightarrow \int_{N_0}^{N(t)} \frac{dN'}{N'} = \int_0^t -k\,dt'$$

$$\Rightarrow \ln N(t) - \ln N_0 = -kt - (-0) \Rightarrow N(t) = N_0 e^{-kt}$$

Thought: For $A + B \to C$, by that logic the rate doubles if I double the concentr. of A or the concentr. of B. So,

$$\frac{\partial [C]}{\partial t} \sim [A]\cdot[B] \quad \text{or,}$$

if $A = B$ so $2A \to C$

$$\frac{\partial [C]}{\partial t} \sim [A]^2$$