L1 : The math of pchem :

① Average

ex: y_i = 1, 2, 3, 3, 4, 4   N = 6 $i = 1 \dots 6$

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

$$= \frac{1}{6}\times 1 + \frac{1}{6}\times 3 + \frac{1}{6}\times 2 + \dots$$

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

↑ P_i Probability   ↑ y_i value.

$y_i \Rightarrow y(x)$

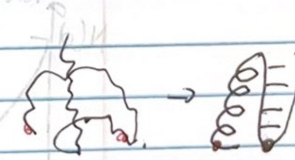
$$\bar{y} = \sum_i P_i y_i = \int P(x)\, y(x)\, dx$$

integration = "continuous summation"

Example: Single molecule reaction

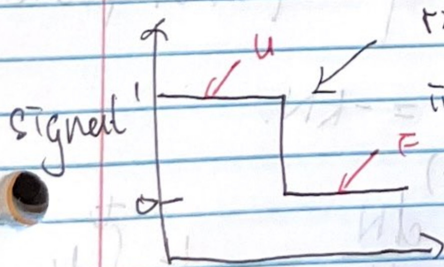
protein folding $U \longrightarrow F$

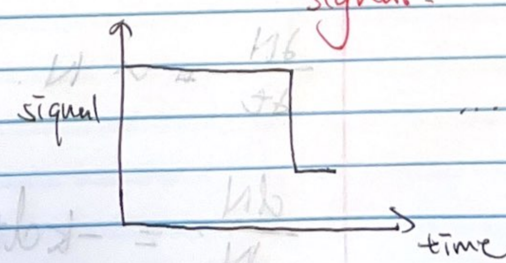
unfolded   Folded



signal

rx is almost "instantaneous"

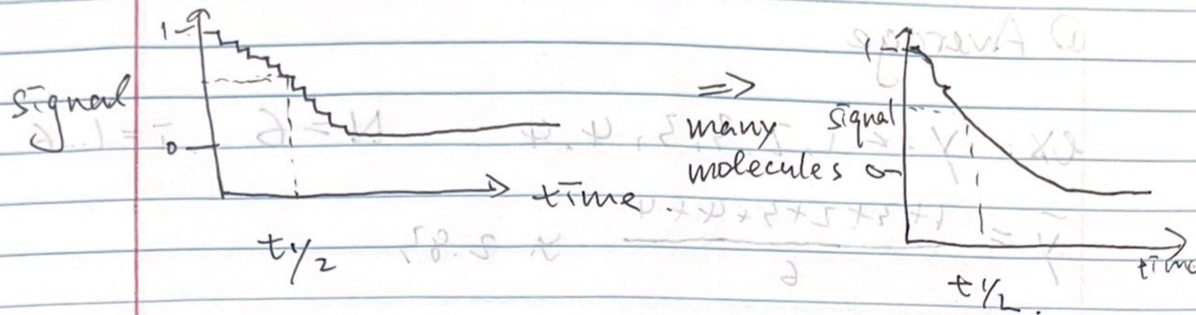




...

⇓

Average.



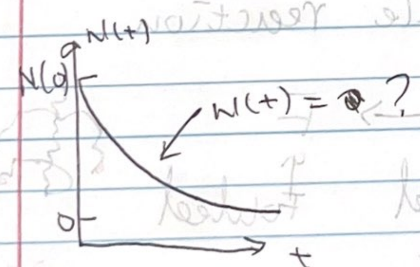
② Derivative model. eg: $\frac{dx}{dt} = f(x,t)$.

↓ solve?

$x(t)$.

The Irony: chemical systems are ~~chemical~~ discrete (moleculy) so ~~real~~ really, it is $\frac{\Delta x}{\Delta t}$, and $\frac{dx}{dt}$ is the approximation.

Example: Start with many ($N(t=0) \gg 1$) protein. How many are left unfolded at time t?



Thought: The rate at which unfolded protein fold is propotional to the number of unfolded proteins.

$$\frac{dN}{dt} \propto N. \quad \text{or} \quad \frac{dN}{dt} = -kN.$$

$$\frac{dN}{N} = -k\,dt. \Rightarrow \int_{N(0)}^{N(t)} \frac{dN}{N} = -k \int_0^t dt$$

$\ln \frac{1}{x} = -\ln x$

$\ln[N(t)] - \ln[N(0)] = -kt$

Taking exponential e^{y} on both sides

$N(t) = N(0) \cdot e^{-kt}$

Ex: For $A + B \rightarrow C$

$$\frac{d[C]}{dt} \propto [A][B]$$