STOCHASTIC SIMULATION ALGORITHM

(D.T. GILLESPIE, J. Phys. Chem 81, 2340 (1977)).

V: VOLUME

SPECIES : $S_1, \dots S_N$

\# OF S_i : X_i

STATE : $(X_1 \dots X_N)$

REACTIONS : R_μ

E.G. R_1: $X_1 \to X_3$, R_2: $X_1 + X_2 \to \dots$, R_3: $X_1 + X_1 \to \dots$

$c_\mu dt$: PROB. FOR A SPECIFIC COMBINATION OF MOLECULES TO REACT ACCORDING TO R_μ

WELL-MIXED, MEMORYLESS SYSTEM

$a_\mu dt$: PROB. FOR R_μ IN $(t, t+dt)$ IF THE SYSTEM IS IN STATE $(X_1 \dots X_N)$ AT t.

R_1: $a_\mu dt = X_1 c_\mu dt$

R_2: $a_2 dt = X_1 \cdot X_2 c_2 dt$

R_3: $a_3 dt = \frac{1}{2} X_1 (X_1 - 1) c_3 dt$

(Q: How is c_μ related to the deterministic rate constants)

$k_1 = c_1$, $k_2 = V c_2$, $k_3 = V c_3 / 2$

SIMULATION:

INITIALIZE : $t = 0$, STATE $(X_1, \dots X_N)$

what is the next reaction?

when does it occur?

=> Pick R_μ, t_μ

=> update state

$P(t,\mu)dt$: Prob. that next reaction in V will occur in $(t, t+dt)$ in V if state is $(X \dots X_N)$ at $t=0$.

$$P(t,\mu)dt = \underbrace{P(T > t)}_{\text{Prob. FOR } \underline{\text{NO}} \text{ RXN IN } [0,t)} \; \underbrace{a_\mu dt}_{\text{PROB FOR } R_\mu \text{ IN } dt}$$

What is $P(T > t)$?

$$P(T > t + dt) = P(T > t)\left(1 - \sum_{1}^{N} a_\nu dt\right) \qquad a = \sum_\nu a_\nu$$

$$P(T > t + dt) = P(T > t)(1 - a dt)$$

$$\frac{P(T > t + dt) - P(T > t)}{dt} = - P(T > t) a \implies P(T > t) = e^{-at}$$

$$\implies \underline{P(t, \mu)^{dt} = e^{-\sum_{\mu=1}^{n} a_\mu t} a_\mu dt}$$

NEXT REACTION:

$$P_\mu = \int_0^\infty dt\, a_\mu e^{-at} = \frac{a_\mu}{a}$$

$$r_1 \in [0,1] \qquad \sum_{\nu=1}^{\mu-1} \frac{a_\nu}{a} < r_1 \leq \sum_{\nu=1}^{\mu} \frac{a_\nu}{a}$$

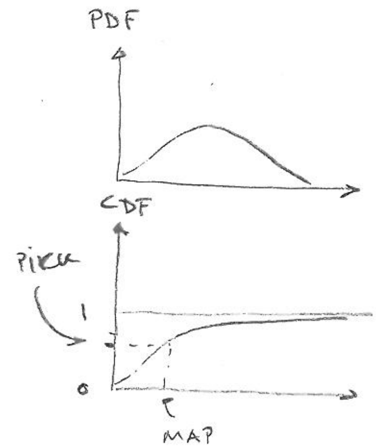
REACTION TIME (ANY REACTION)

$$\sum_\mu a_\mu e^{-at}\, dt = a e^{-at}\, dt$$

CUMULATIVE DISTRIBUTION

$$\int_0^t dt'\, a e^{-at'} = 1 - e^{-at} = r_2 \in [0,1]$$

$$\Rightarrow 1 - r = e^{-at} \Rightarrow \ln(1-r) = -at \Rightarrow t = -\frac{1}{a}\ln(1-r)$$



"INVERSE TRANSFORM SAMPLING" (SMIRNOFF TRANSFORM)

SSA:

0. INITIAL COND.: STATE $(x_1 \ldots x_N)$, RXN RATES k_μ
1. CALCULATE a_μ, a_0
2. GENERATE RANDOM NBRS $r_1, r_2 \Rightarrow$ CALCULATE t, μ
3. UPDATE TIME $t_{i+1} = t_i + t$, STATE (ADJUST NUMBERS ACCORDING TO R_μ)