#10 CTMC

[Andrey Markov 1856 - 1922
Russian Mathematician
lots of things Named after him]

①

[see also Richard Hamming, You and Your Research]

Given $\langle e^{-\Sigma} \rangle = 1$, then $P(\Sigma \leq \varepsilon) \leq e^{+\varepsilon}$ Jarzynski inequality
[alternative derivation]

Markov's inequality $P(x \geq a) \leq \frac{\langle x \rangle}{a}$ for $x \geq 0$

$$\langle x \rangle = \int_{-\infty}^{+\infty} dx\, P(x)\, x = \int_{0}^{+\infty} dx\, P(x)\, x \quad \text{because } x \geq 0$$

positive

$$= \int_0^a dx\, P(x)\, x + \int_a^{\infty} dx\, P(x)\, x$$

$$\geq \int_a^{\infty} dx\, P(x)\, a = a\, P(x > a)$$

[citation needed]

Cernoff bound

$$P(x \geq a) \leq \underbrace{M_x(t)}_{\langle e^{+tx} \rangle} e^{-ta} \qquad t \geq 0$$

moment generating function

$$P(x \geq a) = P(e^{tx} \geq e^{ta}) \quad \text{with } t > 0$$

$$\leq \frac{\langle e^{tx} \rangle}{e^{ta}}$$

Markov's inequality

$$P(\Sigma \leq \varepsilon) = P(e^{t\Sigma} \geq e^{t\varepsilon}) \qquad t < 0$$

$$\leq \langle e^{t\Sigma} \rangle e^{-t\varepsilon}$$

$$\leq e^{\varepsilon} \qquad t = -1$$

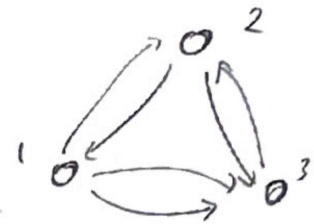
CTMC : trajectory view

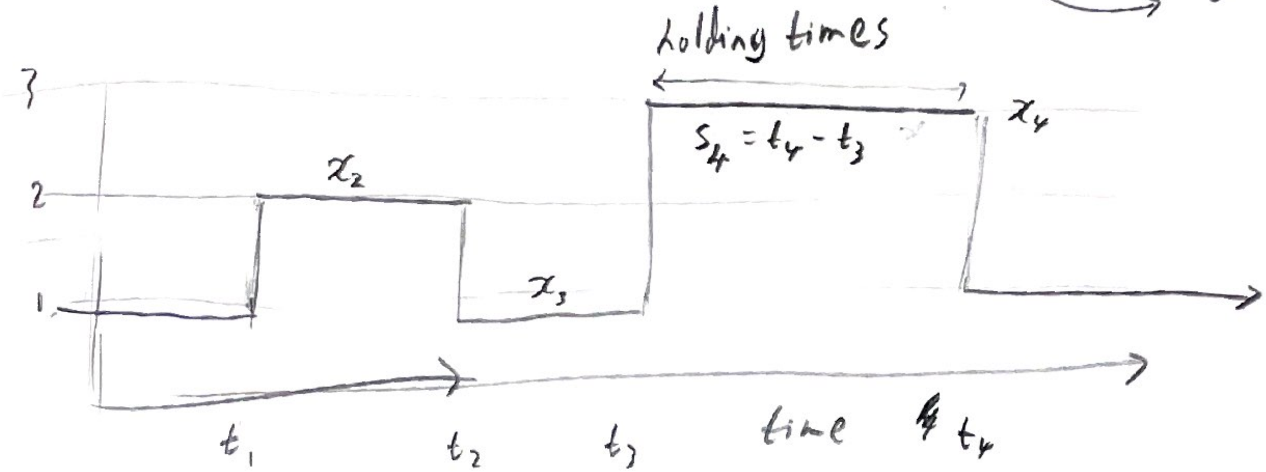
Chain

discrete vs continuous
chain vs process

3

Continuous time Markov Chain CTMC





Jump chain x_1 x_2 x_3

[example: reactions]

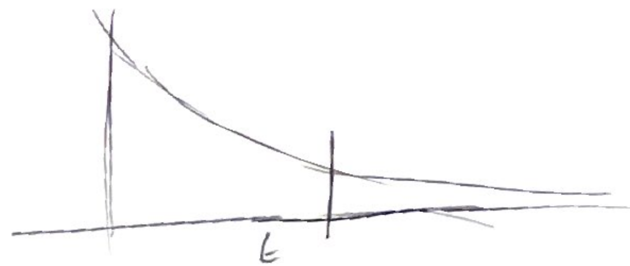
Kolmogorow 1931
Feller 1940
Gillespie 1977

Holding times $\quad$ λ rate $\quad$ mean $\langle x \rangle = \frac{1}{\lambda}$

Holding times - Markov, memorylessness (if there were memory $I(\text{env}:\text{sys}) \neq 0$)

Survival function $s(t) = P(x>t)$

$$P(x>t+s \mid x>t) = P(x>s)$$



$$Exp(x;\lambda) = \lambda e^{-\lambda x}$$

$$S(x;\lambda) = e^{-\lambda x}$$

$$\frac{\int_{t+s}^{\infty} dx\, \lambda e^{-\lambda x}}{\int_{t}^{\infty} \lambda e^{-\lambda x}} \qquad \frac{e^{-(t+s)x}}{e^{-tx}} = e^{-sx} = P(x>s)$$

Exponential & Geometric $\quad$ <u>Only</u> distributions that are memoryless

<u>Proof</u>

$$S(t+s) = s(t)s(s) \qquad s(\tau) = s(1)^{\tau} = e^{\tau \ln s(1)} = \underline{e^{-\lambda \tau}}$$

Leave for next ⇒

Jump chain $\quad J_{ji} = P(x_i \to x_j)_{n+1}$ given a jump has occurred

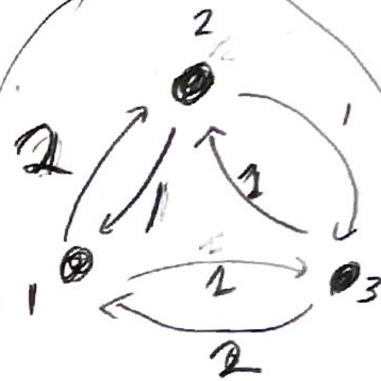
$$P(x_{n+1}) = J\, P(x_n)$$

[note right convention]

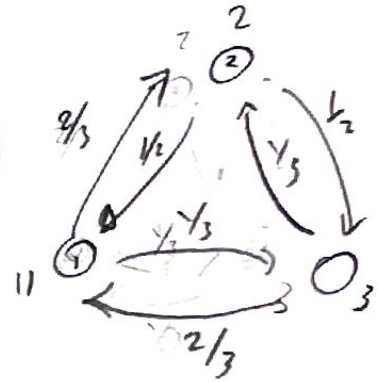
$$J_{ji} \geq 0$$

$$\sum_j J_{ji} = 1$$

* $\quad J_{ii} = 0$



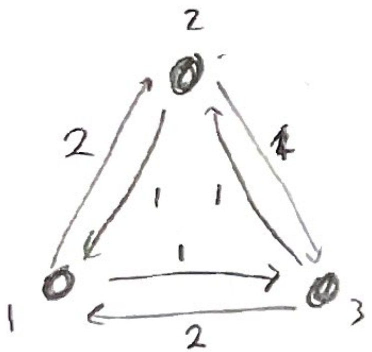
$$\begin{array}{cc} & \qquad\qquad \downarrow \text{in} \\ \text{out} & J = \begin{pmatrix} 0 & 1/2 & 2/3 \\ 2/3 & 0 & 1/3 \\ 1/3 & 1/2 & 0 \end{pmatrix} \end{array}$$

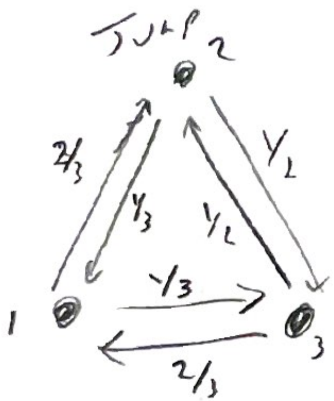


$$Q = \begin{pmatrix} -3 & 1 & 2 \\ 2 & -2 & 1 \\ 1 & 1 & -3 \end{pmatrix}$$

Transition Rate Matrix Q

Rates





$$P(x;t) = e^{+tQ} P(x;0)$$

$$\left.\frac{dP}{dt}\right|_{t=0} = \left.\left[\frac{d}{dt}\sum_n \frac{t^n Q^n}{n!}\right] P(x;0)\right|_{t=0}$$

$$= Q e^{tQ} P(x;0)$$

In

$$\begin{array}{cc} & \\ Q = & \text{out} \begin{pmatrix} -3 & 1 & 2 \\ 2 & -2 & 1 \\ 1 & 1 & -3 \end{pmatrix} \end{array}$$

$$J = \begin{pmatrix} 0 & 1/2 & 2/3 \\ 2/3 & 0 & 1/3 \\ 1/3 & 1/2 & 0 \end{pmatrix}$$

$$\frac{dP}{dt} = QP$$

Master Equation.

off diagonal ≥ 0

$$Q_{ii} = \sum_j Q_{ji}$$

$$J_{ji} = \frac{-Q_{ji}}{Q_{ii}}$$

$$P_H(s|i) = e^{-\lambda s} \qquad \lambda = -Q_{ii}$$

Holding Times

$$p_t = e^{tQ} p_0$$

$$\frac{dp}{dt} = Qp$$

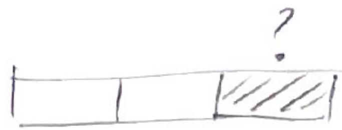
$$M(t) = e^{tQ} \qquad M(0) = I$$

$$\frac{dM(t)}{dt} = Q\,M(t) = M(t)\,Q$$ Kolmogorov forward/backward equations

$$M(t+s) = M(t)\,M(s)$$ Chapman-Kolmogorov eq

(Markov)

t



Trajectory Picture / phase space / state space

$P[X]$ $\qquad \frac{d}{dt}P = QP$ $\qquad x_n \to x_{n+1} \to$

Gillespie

$$P(i \xrightarrow{t} j) = \left[I + Qt + \frac{Q^2 t^2}{2!} \dots \right]_{ji,\ t \to 0}$$

$$= \delta_{ij} + Q_{ji} t + O(t^2)$$

$$P(i \xrightarrow{t} i) = 1 - \lambda_i t + O(t^2)$$

$$P(i \to j)_{j \neq i} = Q_{ji} t + O(t^2)$$

tim

Time Reversal

$M(t)\pi = \pi \qquad Q\pi = 0$

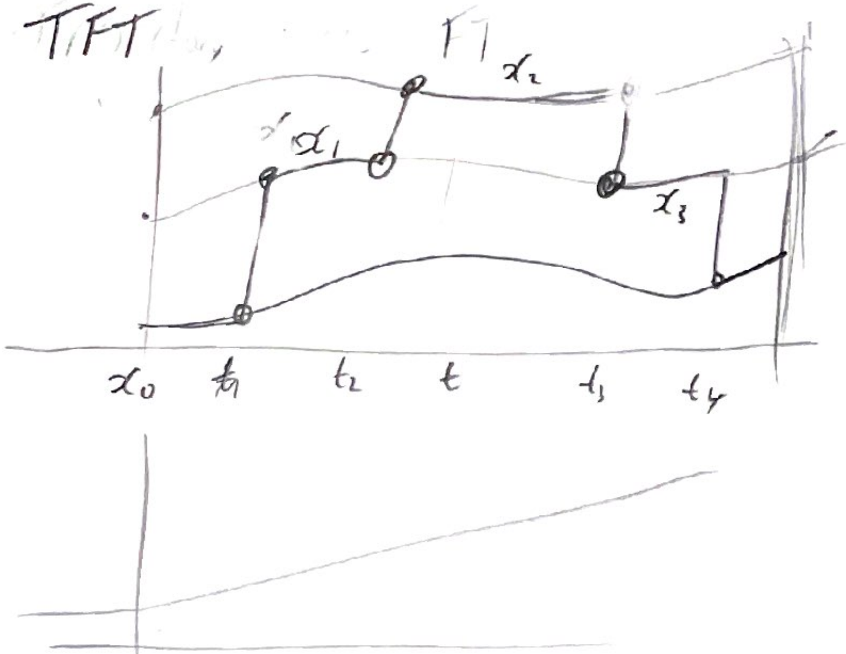
$$\tilde{M} = \mathrm{diag}(\pi)\, M^T\, \mathrm{diag}(\pi^{-1})$$

$$= \mathrm{diag}(\pi) \left[\sum_n \frac{t^n {Q^T}^n}{n!} \right] \mathrm{diag}(\pi^{-1})^{-1} = e^{t\tilde{Q}}$$

$$\tilde{Q} = \mathrm{diag}(\pi)\, Q^T\, \mathrm{diag}(\pi)^{-1}$$

[Does not change holding times]

Trajectory Fluctuation Theorem



$$P[X|x_0] = \prod_{n=0}^{J-1} P_H(x_n)\, P_J(x_n \to x_{n+1}, t_{n+1})$$

$$P_H = e^{-\int_{t_n}^{t_{n+1}} \lambda(\tau)\, d\tau}$$

$$\frac{P[X|x_0]}{P[\tilde{X}|x_t]} = \prod \underbrace{\frac{P_J(x_n \to x_{n+1}, t_{n+1})}{\tilde{P}_J(x_{n+1} \to x_n, t_{n+1})}} = \frac{\tilde{\pi}_n(x_n)}{\tilde{\pi}_{n+1}(x_{n+1})}$$

Jumps are detailed balance.

$$\prod = e^{-\beta \Delta E}$$

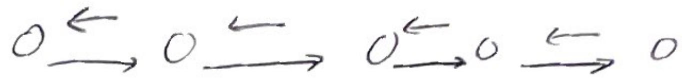
$$= e^{+}$$

$$= e^{-\beta Q[X]}$$ for trajectory.

Dragged Particle on a Ring

~~Action~~ $A = \underbrace{\frac{1}{2}(A+\tilde{A})}_{\Theta} + \underbrace{\frac{1}{2}(A-\tilde{A})}_{\Sigma}$ $\qquad A'$

$$P[x] = e^{-A[x]}$$



$$\begin{pmatrix} -\lambda_R-\lambda_L & \lambda_L & \\ \lambda_R & -\lambda_R-\lambda_L & \\ 0 & \lambda_R & - \\ 0 & 0 & \\ \lambda_L & 0 & \end{pmatrix}$$

$$\frac{K_+}{K_-} = e^{\beta \Delta E}$$

$\langle \Theta_R \rangle$ = Poisson Rate

$\Theta_R = t K_R = \langle n_R \rangle$

$$P(n_R) = \frac{\Theta_R^{n_R}}{n_R!} e^{-\Theta_R}$$

$$P(n_L) = \frac{\Theta^{n}}{n!}$$

$$P(n) = P(n_R - n_L)$$

Modified Bessel function 1st Kind

$$P(n) = e^{-(\Theta_L + \Theta_R)} \left(\frac{\Theta_R}{\Theta_L}\right)^{n/2} I_n\left(2\sqrt{\Theta_R \Theta_L}\right) \quad A2$$

Skellam distribution

mean $\Theta_R - \Theta_L$ ← all odd cumulants

var $\Theta_R + \Theta_L$ ← all odd cumulants.

Poisson, all cumulants $K_n = \Theta \quad K_1 = \Theta$

$$\frac{P(+n)}{P(-n)} = e^{n \ln \frac{\Theta_R}{\Theta_L}}$$

$$I_n(x) = I_{-n}(x)$$

$$\ln \frac{\Theta_R}{\Theta_L} = \ln \frac{K_R}{K_L} = \text{entropy production per transition}$$

$$= e^{-\beta \Delta E} \quad \Delta E \quad e^{-\beta(E_R - E_L)}$$

"A month in the library can often save an hour in the library"

Frank Westheimer