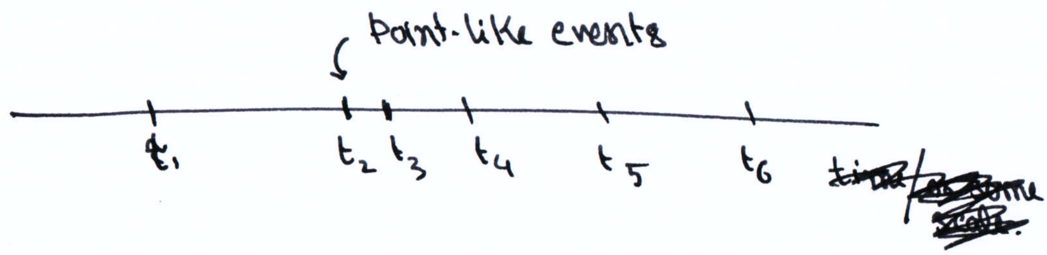
~~Stochastic processes~~ few definitions

① **Point process:** (a sequence of events)



Ex: photon counter, earthquakes, neural spikes etc.

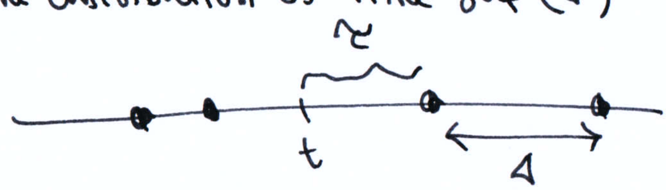
- A hot topic: determinantal point process: Prob as determinant of something.

  Ex: Eigenvalues of Random matrix

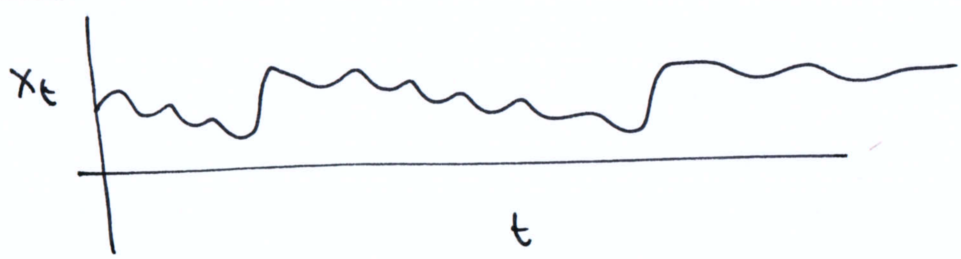
- Waiting time and renewal theory.

  ① What is the distribution of time before an event happens. (τ)

  ② What is the distribution of time-gap (Δ)

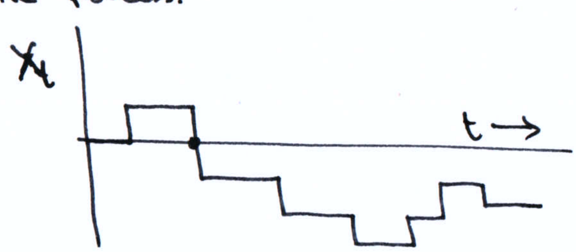


② **Stochastic process:**



Formal ~~Mathematical~~ definition: let η is a random variable with prob $P(\eta)$. then, a mapping $\eta \to X_t$ is called realization of a stochastic process.

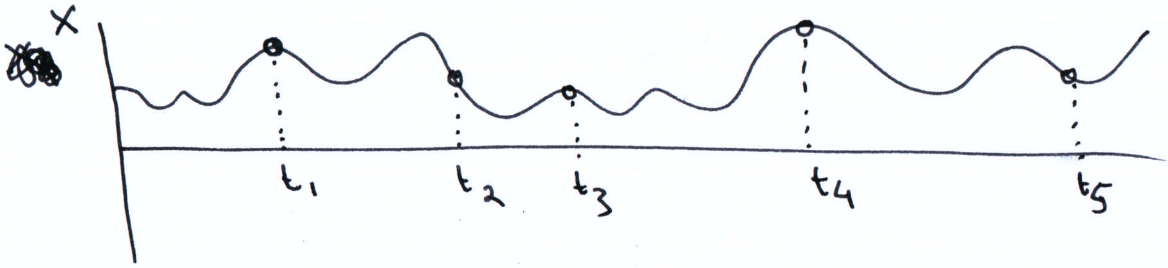
Example: Random walk



jumps are from η.

Think like a dynamicist. -

Markov- stochastic process : Book by van Kampen



If conditional probability

$$M(x_{n+1}, t_{n+1} \mid x_n, t_n; \cdots; x_1, t_1) = M(x_{n+1}, t_{n+1} \mid x_n, t_n)$$

Then Markovian. (Also called transition probability)

Remark: The dynamics is completely characterized by the Conditional probability $M(x_{n+1}, t_{n+1} \mid x_n, t_n)$. and initial ~~condi~~ probability.

Remark: Note, how time scale is important.

$$P(x_{n+1}, t_{n+1}; x_n, t_n) = M(x_{n+1}, t_{n+1} \mid x_n, t_n)\, P(x_n, t_n)$$

Repeating

$$P(x_{n+1}, t_{n+1}; x_n, t_n; \cdots; x_1, t_1) = M(x_{n+1}, t_{n+1} \mid x_n, t_n)\, M(x_n, t_n \mid x_{n-1}, t_{n-1}) \cdots M(x_1, t_1 \mid x_0, t_0)\, P(x_0, t_0)$$

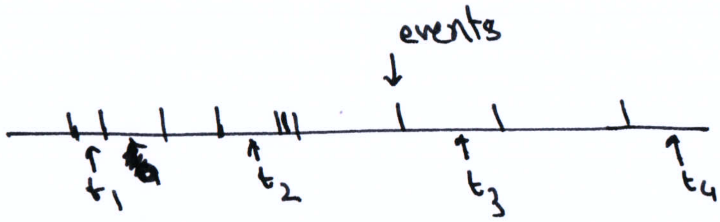
⊛ **Show:**

$$\boxed{M(x_{n+1}, t_{n+1} \mid x_{n-1}, t_{n-1}) = \int dx_n\, M(x_{n+1}, t_{n+1} \mid x_n, t_n)\, M(x_n, t_n \mid x_{n-1}, t_{n-1})}$$

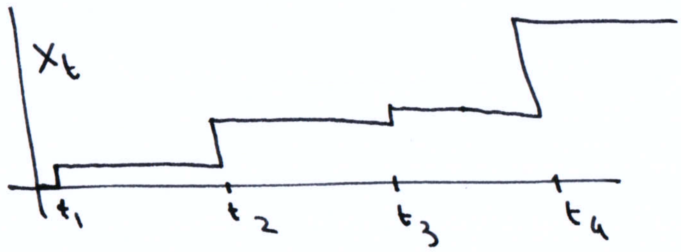
Chapman- Kolmogorov equation.

Examples of Markov process:

(a) Poisson process:



let X_{t_1} = total number of events up to time t_1.



$$M(x_{n+1}, t_{n+1} | x_n, t_n) = \frac{[\lambda(t_{n+1}-t_n)]^{x_{n+1}-x_n}}{(x_{n+1}-x_n)!} e^{-\lambda(t_{n+1}-t_n)}$$

$\lambda :=$ rate of event.

Example: radioactive decay.

(b) Wiener-Process / Brownian motion

$$M(x_{n+1}, t_{n+1} | x_n, t_n) = \frac{1}{\sqrt{2\pi D(t_{n+1}-t_n)}} e^{-\frac{(x_{n+1}-x_n)^2}{2D(t_{n+1}-t_n)}}$$

Example of non-Markov process: fractional Brownian motion.

$$P[x(t)] \sim e^{-\int dt_1 dt_2 \, x(t_1) c^{-1}(t_1,t_2) x(t_2)}$$

with $c(t_1,t_2) = t_1^{2H} + t_2^{2H} - |t_1-t_2|^{2H}$

Stationary Markov process:

$$M(x',t'|x,t) = M(x',t'-t|x,0)$$

⊛ There is subtlety in exact definition. For details see van Kampen.

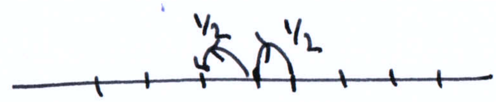
~~called a homogeneous Markov process.~~

Markov chain:

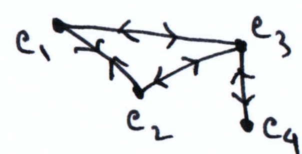
A stationary Markov process, on discrete time $\{0,1,2,\ldots\}$ and discrete space X.

Not a strict definition

Example random walk



Few basic properties of Markov chains



⊛ Time-homogeneous Markov chain:

$$M(e',t|e,0) = M(e',e)$$

does not depend on time.

⊛ $$P_{t+\Delta t}(e') = \sum_{e} M(e',e)\,P_t(e)$$ Master-equation.

~~Properties of~~ ~~In vector notation~~

in operator notation: $|P_{t+\Delta t}\rangle = M|P_t\rangle$

$$|P_t\rangle = \begin{pmatrix} P_t(e_1) \\ \vdots \\ P_t(e_n) \end{pmatrix} \qquad M = \begin{pmatrix} & & \\ & M(e',e) & \\ & & \end{pmatrix}$$

Easy reference: ① Sethna Book, ch 8.2
② van Kampen.

Basic properties of M:

① $\boxed{M(c'|c) \geq 0}$ ~~[illegible]~~. (because they are probability)

② Conservation of probability gives

$$1 \Leftarrow \sum_{c'} P_{t+\Delta t}(c') = \sum_{c} \underbrace{\left(\sum_{c'} M(c',c) \right)}_{1} P_t(c)$$

$$= \sum_{c} P_t(c) = 1$$

$\Rightarrow \boxed{\sum_{c'} M(c',c) = 1}$ unit column sums
(Markov-matrix)

~~This is usually incorporated by writing~~

$\cancel{M(c,c) = 1 - \sum_{c' \neq c} M(c',c)}$ ~~in master equation, which~~

~~gives~~

$\cancel{P_{t+\Delta t}(c) = \sum_{c \neq c} \ldots}$

③ M is NOT symmetric! (non-Hermitian)

Means, left and right eigenvectors are not same.

For each eigenvalue λ:

$$M|r_\lambda\rangle = \lambda |r_\lambda\rangle \quad \text{and} \quad \langle l_\lambda| M = \lambda \langle l_\lambda|$$

Peculiarities:

- λ could be complex number.
- May not be fully diagonalizable (Jordan block decomposition)
- Eigenstates may not form a ~~[illegible]~~ complete set — Example: TS & Deepak Dhar, J Stat phys.

Interesting reading: Hermitian is not self-adjoint.
For QM example, see a phys today article.

~~Stationary state~~ : at ~~large~~ time.

$$~~|P_{t+\Delta t}\rangle = |P_t\rangle = |P_{st}\rangle~~$$

Expressing in terms of eigenbasis :

$$\sum_\lambda |r_\lambda\rangle\langle l_\lambda| = \mathbb{1}_{N\times N}$$

$$\langle l_\lambda | r_{\lambda'}\rangle = \delta_{\lambda,\lambda'}$$

Completeness

Orthonormality.

We write

$$|P_t\rangle = \sum_\lambda \langle l_\lambda|P_t\rangle \cdot |r_\lambda\rangle$$

Then, time evolution gives,

$$|P_t\rangle = M\,|P_{t-\Delta t}\rangle = M^2\,|P_{t-2\Delta t}\rangle$$

$$= M^n\,|P_0\rangle$$

$$= M^n \sum_\lambda \langle l_\lambda|P_0\rangle\,|r_\lambda\rangle$$

$$= \sum_\lambda \langle l_\lambda|P_0\rangle\,\lambda^n\,|r_\lambda\rangle$$

Stationarity: If there is a time independent state at $t\to\infty$, then ① that state corresponds to $\lambda = 1$.

② And rest $|\lambda| < 1$.

③ and $\langle l_1| = \langle 1|$ because $\sum_{c'} M(c',c) = 1$

$$\Rightarrow \langle 1|M = \langle 1|$$

④ $|P_t\rangle \xrightarrow[t\to\infty]{} |P_{st}\rangle = |r_1\rangle$

The right eigenvector associated to largest eigenvalue gives stationary state.

Q. What ensures stationarity?

Perron-Frobenius theorem: Let M be an irreducible, non-negative square matrix, (with period 1), then

① Largest eigenvalue λ_0 is real and positive. $\lambda_0 \geq 0$.

② Rest eigenvalues $|\lambda| < \lambda_0$.

③ Largest eigenstate is non-degenerate, meaning there is exactly one right eigenvector (r_0) and one left eigenvector (l_0).

④ All elements of r_0 and l_0 are positive (>0). And they are the only such eigenvectors.

(*) Irreducible essentially means: if M has some zero entries, then M^n has all positive elements for finite n.

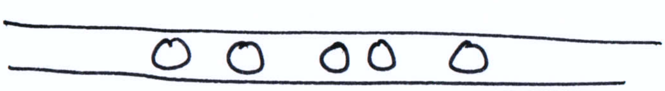
Example: $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ is reducible, $\Rightarrow$ No Perron-Fro. Th.

(*) Irreducible M means, ergodic. $\Rightarrow$ it is possible to go from one state to another by finite steps.

Example of a reducible (non-ergodic) matrix M:

$$M = \begin{pmatrix} [A] & 0 \\ 0 & [B] \end{pmatrix}$$ block diagonal.

Example of such a dynamics $\longrightarrow$ energy conserving moves.



Elastic collison. Only two energies E_1, E_2

⊛ Recall the standard definition of irreducible matrix.

that M can not be transformed into a upper block triangular form by PMP^{-1}, where P is a permutation matrix.

How is this related to the definition we used?

Ans: Hint: permutation means relabelling of states.

Periodicity: $M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Rightarrow \lambda = 1$ degenerate.

check: $\left.\begin{array}{l} M^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ M^3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = M \end{array}\right\} \Rightarrow$ ergodic/irreducible.

what it means? The ~~config~~ system jumps from one config to another and back periodically.

$(1\,0) \to (0\,1) \to (1\,0) \to (0\,1)$

$\Rightarrow$ Period $= 2$.

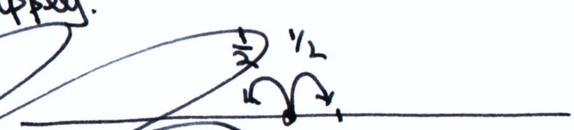
Means, ergodic, but still no unique stationary state.

~~Rem Remark: An example where PF does not apply.~~

~~Random walk~~

Remark: An example where PF does not apply.

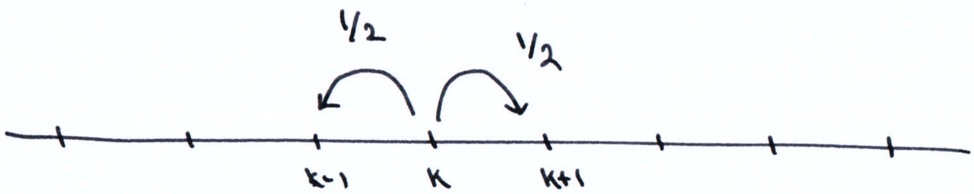
Random walk on an infinite line.



~~MOO~~

$\Big($

An example where PF does not apply.



$$P_{t+\Delta t}(k) = \frac{1}{2}\left[P_t(k-1) + P_t(k+1)\right]$$

$$\Rightarrow \ |P_{t+\Delta t}\rangle = \mathcal{M}\,|P_t\rangle \quad \text{with} \quad \mathcal{M} = \begin{pmatrix} \ddots & & & & & \\ & \ddots & & & & \\ & \frac{1}{2} & 0 & \frac{1}{2} & & \\ & & \frac{1}{2} & 0 & \frac{1}{2} & \\ & & & & \ddots & \\ & & & & & \ddots \end{pmatrix}$$

because it is infinite.

(we solve this problem soon). (There is no stationary state!)

But, PF applies if it is on a periodic boundary.

$$\mathcal{M} = \begin{pmatrix} 0 & \frac{1}{2} & 0 & \cdots & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & \cdots & \\ 0 & & \ddots & & & \\ \vdots & & & & \ddots & \frac{1}{2} \\ \frac{1}{2} & 0 & & 0 & \frac{1}{2} & 0 \end{pmatrix} \quad \text{Finite matrix.}$$

There is a unique stationary state. where all sites are equally probable.

Easy to see: $\mathcal{M}$ is symmetric. $\Rightarrow |l_0\rangle \equiv |r_0\rangle$

we know $|l_0\rangle = |1\rangle \Rightarrow |r_0\rangle = |1\rangle$.

<u>Remark</u>: PF is related to phase transition in equilibrium. Phase transitions happen when PF does not apply for transfer matrix.

<u>Ref</u>: Cuesta & Sánchez, J Stat Phy (2004).
Sanyal, Klamser, Sadhu, Dhar, PRL (2018).

Continuous time process (but state space discrete)

$$M(c',c) = \delta_{c',c} + \Delta t\, \omega(c',c) + O(\Delta t^2)$$

$$\Rightarrow \quad P_{t+\Delta t}(c') = \sum_c M(c',c) P_t(c)$$

$$= \sum_c \left[\delta_{c',c} + \Delta t\, \omega(c',c) + \cdots\right] P_t(c)$$

$$= P_t(c') + \Delta t \sum_c \omega(c',c) P_t(c) + O(\Delta t^2)$$

$$\Rightarrow \quad \frac{P_{t+\Delta t}(c') - P_t(c')}{\Delta t} = \sum_c \omega(c',c) P_t(c) + O(\Delta t)$$

in $\Delta t \to 0$ limit

$$\boxed{\frac{dP_t(c')}{dt} = \sum_c \omega(c',c) P_t(c)}$$

Master equation,

OR

Pauli-M-equation,

$$\boxed{\frac{d|P_t\rangle}{dt} = W|P_t\rangle}$$

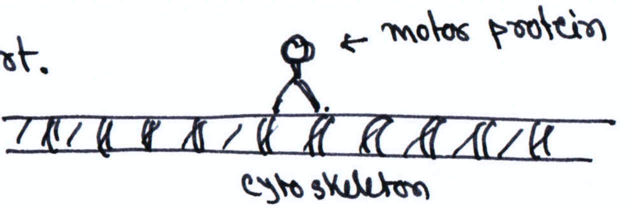
Rate equation.

Remark: $\omega(c',c) =$ is transition rate, therefore can be larger than 1.

$\Delta t \cdot \omega(c',c)$ gives the probability of a transition for small Δt.

Remark: $\omega(c',c)$ can be computed ~~[illegible]~~ or measured ~~for a given~~ from the dynamics of a given system.

Example. Biological transport.



Example: chemical reactions

$$A + B \longrightarrow C$$

Example: transport of ion in hydrogen bonded network.

extra ion. (hydronium ion)

Grotthuss mechanism.

[TS. arXiv; 1009]

Example: Fermi's golden rule in QM.

time-dependent perturbation theory gives, ~~to~~.

$H_{system} + H_{extern.}$ ← perturbation.

↳ E_n are eigen states of H_{system}

$$W(n', n) = \frac{2\pi}{\hbar} \left| H_{Ext}(n', n) \right|^2 \rho(E_n)$$

matrix element in E_n basis.

density of states.

Remark: ① spot the difference of $\frac{d|P_t\rangle}{dt} = W|P_t\rangle$ with Sch equation

$$i\hbar \frac{d}{dt}|\psi_t\rangle = H|\psi_t\rangle$$

② Compare with Boltzmann equation. See that B-equation is non-linear in phase space density, but M-equation is linear in P.

(*) A conventional form of the M-equation.

$$\sum_{c'} M(c',c) = 1$$

$$\Rightarrow \quad 1 + \Delta t \sum_{c'} w(c',c) + \dots = 1 \quad \Rightarrow \quad \boxed{\sum_{c'} w(c',c) = 0}$$

Column sum of W-matrix vanish.

A natural choice

$$w(c,c) = -\sum_{c' \neq c} w(c',c) \qquad \text{along the diagonal.}$$

$$W = \begin{pmatrix} \ddots & & w_1 & & \cdots \\ & \ddots & w_2 & & \\ & & -\sum w_i & & \\ & & w_N & \ddots & \\ \cdots & & \vdots & & \ddots \end{pmatrix}$$

Typically, this is incorporated in the M-equation by writing

$$\frac{d}{dt} P_t(c') = \sum_{c \neq c'} w(c',c)\, P_t(c) + w(c',c')\, P_t(c')$$

$$\downarrow$$

$$- \sum_{c'' \neq c'} w(c'',c')\, P_t(c')$$

$\downarrow$ c'' is dummy variable then, call it c.,

$$- \sum_{c \neq c'} w(c,c')\, P_t(c')$$

$$= \sum_{c \neq c'} \left[w(c',c)\, P_t(c) - w(c,c')\, P_t(c') \right]$$

for c=c', is zero. so we can write

$$\boxed{\frac{d}{dt} P_t(c') = \sum_{c} \left[w(c',c)\, P_t(c) - w(c,c')\, P_t(c') \right]}$$