Recorrência

$T^{\ell}(\overleftarrow{n,m})$: probabilidade de ir de "m" para "n" em "ℓ" passos.

→ todos os possíveis caminhos incluindo os que passam por "n" antes de "ℓ" passos.

$R_\ell(n,m)$: prob. de passar pela 1ª vez por "n" em "ℓ" passos partindo de "m"

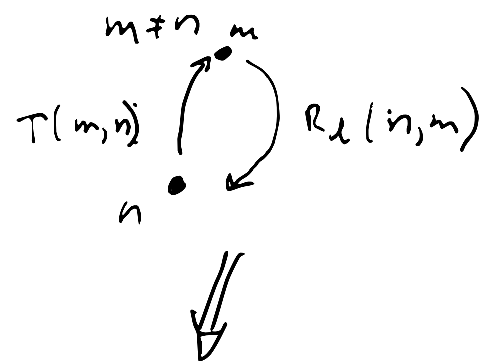
→ Prob. de 1ª passagem

Kac : $$\boxed{T_\ell(n,m) = \sum_{j=1}^{\ell} T_{\ell-j}(n,n)\, R_j(n,m)} \quad (*)$$

$T_j(n,m) = T^j(n,m)$ se $j \neq 0$

$\ell \geq 1$

$T_0(n,m) = \delta_{nm}$



Propriedades:

$$T_0(n,n) = 1$$

$$T_1(n,m) = T(n,m)$$

$$R_1(n,m) = T(n,m)$$

$$\boxed{R_{\ell+1}(n,n) = \sum_{m \neq n} R_\ell(n,m)\, T(m,n)}$$

Para resolver (*) definimos as funções geratrizes

$T_0(n,m)$

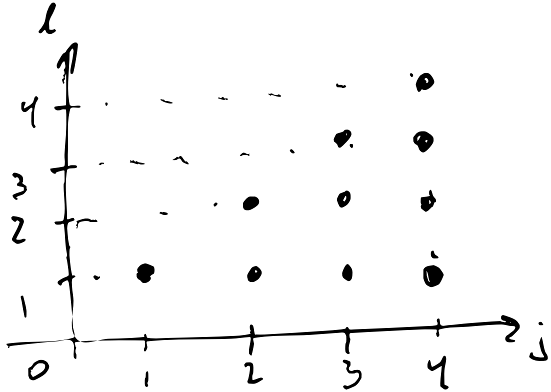
- $$G(n,m,z) = \sum_{l=1}^{\infty} T_l(n,m)\, z^l + \delta(n,m)$$

- $$H(n,m,z) = \sum_{l=1}^{\infty} R_l(n,m)\, z^l$$

(*) $$T_l(n,m) = \sum_{j=1}^{l} T_{l-j}(n,n)\, R_j(n,m)$$

$$\underbrace{\sum_{l=1}^{\infty} T_l(n,m)\, z^l} = \sum_{l=1}^{\infty} \sum_{j=1}^{l} T_{l-j}(n,n)\, R_j(n,m)\, z^l$$

$$G(n,m,z) - \delta(n,m) = \sum_{l=1}^{\infty} \sum_{j=1}^{l} T_{l-j}(n,n)\, z^{l-j}\, R_j(n,m)\, z^j$$



$$\sum_{l=1}^{\infty}\sum_{j=1}^{l} = \sum_{j=1}^{\infty}\sum_{l=j}^{\infty} = \sum_{j=1}^{\infty}\sum_{l-j=0}^{\infty}$$

$$G(n,m,z) - \delta(n,m) = \sum_{l=1}^{\infty}\sum_{j=1}^{l} T_{l-j}(n,n)\, z^{l-j}\, R_j(n,m)\, z^j$$

$$G(n,m,z) - \delta(n,m) = \sum_{j=1}^{\infty}\sum_{l-j=0}^{\infty} T_{l-j}(n,n)\, z^{l-j}\, R_j(n,m)\, z^j$$

$$= \sum_{m=0}^{\infty} T_m(n,n)\, z^m \sum_{j=1}^{\infty} R_j(n,m)\, z^j$$

$$\boxed{G(n,m,z) = G(n,n,z)\, H(n,m,z) + \delta(n,m)}$$

• Se $n \neq m \rightarrow \delta(n,m) = 0$

$$H(n,m,z) = \frac{G(n,m,z)}{G(n,n,z)}$$

• Se $n = m \rightarrow \delta(n,n) = 1$

$$H(n,n,z) = 1 - \frac{1}{G(n,n,z)}$$

Probabilidade de recorrência do estado n:

$$R(n) = \sum_{l=1}^{\infty} R_l(n,n) = \sum_{l=1}^{\infty} R_l(n,n)(1^l)$$

$$= H(n,n,1) = 1 - \frac{1}{G(n,n,1)}$$

$$\boxed{R(n) = 1 - \frac{1}{G(n,n,1)}}$$

- Se $G(n,n,1) \longrightarrow \infty$ então o estado n é recorrente e neste caso podemos calcular o tempo médio de recorrência.

$$\langle \ell \rangle = \sum_{\ell=1}^{\infty} \ell \, R_\ell(n,n) = \frac{d}{dz}\left[\sum_{\ell=1}^{\infty} R_\ell(n,n)\, z^\ell \right]\Bigg|_{z=1}$$

$$\langle \ell \rangle = \lim_{z \to 1} \frac{d}{dz} H(n,n;z)$$

- Se $G(n,n,1)$ é finito, $R(n) < 1$ e o estado n pode não ser atingido novamente.

$\Rightarrow$ Sabemos da expansão em autofunções que

$$T_l(n,m) = \sum_k \lambda_k^l \psi_k(n) \phi_k(m)$$

Da definição de G:

$$G(n,m,z) = \sum_{l=1}^{\infty} T_l(n,m) z^l + \delta(n,m)$$

$$= \sum_{l=1}^{\infty} \sum_k \lambda_k^l \psi_k(n) \phi_k(m) z^l + \lambda_0^0 T_0(n,m) z^0$$

$$= \sum_k \psi_k(n) \phi_k(m) \underbrace{\sum_{l=1}^{\infty} (\lambda_k z)^l}_{|\lambda_k| \le 1}$$

$$1 + \cancel{a} + \cancel{a^2} + \dots + \cancel{a^N} = S$$

$$\cancel{a} + \cancel{a^2} + a^3 + \dots + a^{N-1} = aS$$

$$S - aS = 1 - a^{N-1}$$

$$S = \frac{1 - a^{N-1}}{1-a} \xrightarrow{N \to \infty} \frac{1}{1-a}$$

$$G(n,m,z) = \sum_k \psi_k(n)\, \phi_k(m)\, \frac{1}{1 - z\lambda_k}$$

$$\boxed{G(n,m,z) = \sum_k \frac{\psi_k(n)\, \phi_k(m)}{1 - z\lambda_k}}$$

Para saber se "n" é recorrente

$$G(n,n,z) = \frac{\psi_0(n)\,\phi_0(m)}{1 - z\lambda_0} + \sum_{k\neq 0}{}' \frac{\psi_k(n)\,\phi_k(m)}{1 - z\lambda_k}$$

$$\begin{cases} \psi_0(n) \equiv P_\infty(n) \quad (\text{estacionária}) \\ \phi_0(m) \equiv 1 \quad ; \quad \lambda_0 = 1 \end{cases}$$

$$G(n,n,z) = \frac{P_\infty(n)}{1-z} + \sum_{k=0}{}' \frac{\psi_k(n)\,\phi_k(m)}{1 - z\lambda_k}$$

- Se N é finito, $P_\infty(n) > 0$ (pelo Teor. de Perron - Frobenius) ; $G(n,n,z) \xrightarrow{z \to 1} \infty$

$\rightarrow$ qualquer estado é recorrente!

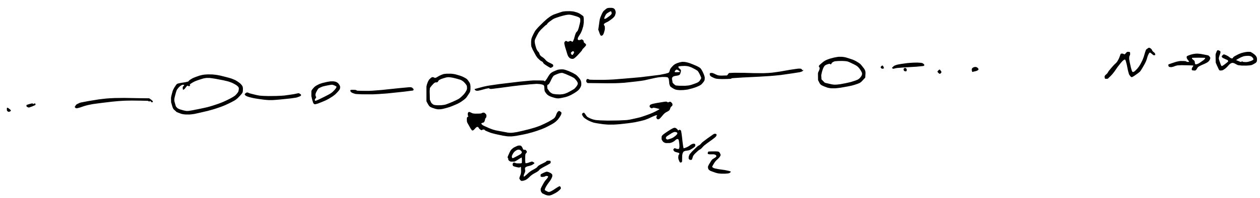
$$G(n,n,z) = P_\infty(n)\,(1-z)^{-1}$$

$$H(n,n,z) = 1 - \frac{1}{G(n,n,z)}$$

$$= 1 - \frac{(1-z)}{P_\infty(n)}$$

$$\langle \ell \rangle = \lim_{z\to 1} \frac{d}{dz} H(n,n,z) = \frac{1}{P_\infty(n)}$$

Recorrência no passeio aleatório (infinito)



→ Condições de contorno periódicas.

$$n = 0, 1, 2, \dots, N-1$$

$$T(m,n): \quad \begin{cases} T(n-1,n) = \dfrac{q}{2} = T(n+1,n) \\ T(n,n) = p \\ T(n,m) = 0, \quad \text{outros casos} \end{cases}$$

$$|P_{\ell+1}\rangle = \hat{T}\,|P_\ell\rangle$$

↓ components

$$P_{\ell+1}(n) = \sum_m T(n,m)\,P_\ell(m) \qquad (A)$$

$$= \frac{q}{2}\,P(n+1) + p\,P(n) + \frac{q}{2}\,P(n-1)$$

↳ Probabilidade estacionária

$$P_\infty(n) = \frac{1}{N}\,;\ \forall n$$

$\hat{T}$ é matriz de TOEPLITZ (diagonais constantes)

$$\begin{bmatrix} a & b & c & d \\ f & a & b & c \\ g & f & a & b \\ h & g & f & a \end{bmatrix}$$

$n-m=-1$

$n-m=0$

$n-m=1$

$$T(n,m) = f(n-m)$$

periódica
(devido às condições)

$$f(n+N) = f(n)$$

→ Para o caso considerado

$$f(1) = f(-1) = \frac{q}{2} \quad ; \quad f(0) = p$$

$$f(m) = 0 \quad , \text{ qualquer outro } m.$$

(A) $$P_{\ell+1}(n) = \sum_m \overbrace{f(n-m)}^{T(n,m)} P_\ell(m)$$

Os autovetores de uma matriz de Toeplitz são sempre

$$\psi_k(n) = \frac{1}{N} e^{ikn} \quad ; \quad k = \frac{2\pi j}{N} \quad ; \; j \in \{0, 1, \dots N-1\}$$

De fato: $\hat{T} |\psi\rangle = \lambda |\psi\rangle$

componentes

$$\sum_m T(n,m)\, \psi_k(m) = \lambda_k \psi_k(n)$$

$$\sum_m' f(n-m) \frac{1}{\cancel{N}} e^{ikm} = \lambda_k \frac{1}{\cancel{N}} e^{ikn}$$

$$\sum_m' f(n-m)\, e^{ik(m-n)} = \lambda_k$$

$$f(-1)\, e^{-ik} + f(0)\, e^{0} + f(1)\, e^{ik} = \lambda_k$$

$$\lambda_k = \frac{q}{2} e^{-ik} + p + \frac{q}{2} e^{ik}$$

$$\lambda_k = p + q \left(\frac{e^{-ik} + e^{ik}}{2} \right)$$

$$\boxed{\lambda_k = p + \cos k}$$

→ Com estes λ_k, a eq. dos autovetores está satisfeita para ψ_k dados.

→ Os autovetores à esquerda são

$$\phi_k(n) = e^{-ikn}$$

Portanto : $T^l(n,m) = \sum_k \lambda_k^l \, \psi_k(n) \, \phi_k(m)$

... VER LIVRO

Voltando a G:

$$G(n,n,z) = \cancel{\frac{P_\infty(n)}{1-z}} + \sum_{k=0}' \frac{\chi_k(n)\,\phi_k(n)}{1-z\lambda_k}$$

$$0 \left(\frac{1}{N} \to 0 \quad \text{se} \quad N \to \infty \right)$$

$$G(n,n,z) = \sum_j' \frac{1}{N} \frac{e^{ikn}\, e^{-ikn}}{1-z\lambda_k} \quad ; \quad \underline{k = \frac{2\pi}{N} j}$$

$$= \frac{1}{N} \sum_j' \frac{1}{1-z\lambda_k} = \frac{1}{N} \sum_j' \frac{1}{1-z(p+q\cos k)}$$

- Se $N \to \infty$: $\sum_j' \to \int dj \to \frac{N}{2\pi} \int dk \;;\; dk = \frac{2\pi}{N} dj$

$$G(n,n,z) = \frac{1}{\cancel{N}} \frac{\cancel{N}}{2\pi} \int_{-\pi}^{\pi} \frac{1}{1-z(p+q\cos k)}\, dk$$

$$G(n,n,z) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{1}{1-z\,(1-q+q\cos k)}\,dk$$

$$= \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{dk}{(1-z)+qz\,(1+\cos k)}$$

Integração fácil: $x = \tan(k/2)$

$\downarrow$

$$\cos k = \frac{1-x^2}{1+x^2}$$

$\vdots$

$$G(n,n,z) = \frac{1}{\sqrt{(1-z)(1-z+2qz)}} \xrightarrow{z\to 1} [1-z]^{-1/2} \to \infty$$

Preciso calcular

$$\mathcal{R}(n) = 1 - \frac{1}{G(n,n,1)}$$

$\sim (1-z)^{-1/2} \xrightarrow{z \to 1} \infty$

Para o caso <u>1D infinito</u> $\mathcal{R}(n) \longrightarrow 1$

↳ qualquer estado é recorrente numa caminhada 1D infinita

Em 2D $\quad \vec{n} = (n_1, n_2)$

$$T(n,m) = \frac{q}{4} \quad \text{se} \quad \begin{array}{l} n_1 = m_1 \pm 1 \\ n_2 = m_2 \pm 1 \end{array} \quad \text{ou}$$

$$T(n,n) = p$$

$\rightarrow$ Condições periódicas em 2D

$$f(\vec{n}) = f(n_1, n_2)$$

$\rightarrow$ $f(\vec{n}) = \frac{q}{4}$ se $|\vec{n}| = 1$

$f(0) = p$

$f(n) = 0$, caso contrário.

↳ Autovalores : $\lambda_k = \sum_{\vec{n}} f(\vec{n})\, e^{i\vec{k}\cdot\vec{n}}$; $\vec{k} = (k_1, k_2)$

$$= p + \frac{q}{2}\left(\cos k_1 + \cos k_2\right)$$

;

$$G(n,n,z) = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{dk_1\, dk_2}{1 - z\lambda_k}$$

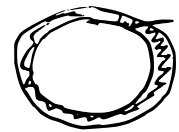
;

$$= \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{dk_1\, dk_2}{(1-z) + qz\left[2 - (\cos k_1 + \cos k_2)\right]}$$

↳ también diverge en una

región próxima a origen $|k| \leq \varepsilon \ll 1$

Próximo à origem $|\vec{k}|<\epsilon$



$2\pi k\, dk$

$$\int \frac{dk_1\, dk_2}{a+k_1^2+k_2^2} = \int_0^{\epsilon} \frac{2\pi k\, dk}{a+k^2} = \pi \ln\left(\frac{a+\epsilon^2}{a}\right)$$

$\left(\frac{1-z}{qz}\right)$

da expansão de

$\cos(k_1)$ e $\cos(k_2)$ próximo a 0

$$\cos(x) = 1 - \frac{x^2}{2} + \dots$$

Se $z \to 1$: $G(n,n,z) = \pi \ln(1-z) \xrightarrow{z\to 1} \infty$

Em 2D também todos os estados são recorrentes

Em d dimensões $\underline{\underline{d \geq 3}}$

⋮

$$G(n,n,z) = \frac{1}{(2\pi)^d} \iint \cdots \int \frac{dk_1\, dk_2 \cdots dk_d}{1 - z\,\lambda_k}$$

$$\lambda_k = p + \frac{q}{d}\left(\cos k_1 + \cos k_2 + \cdots + \cos k_d\right)$$

$z \to 1$:

$$G(n,n,z) = \frac{1}{(2\pi)^d} \iint \cdots \int_{-\pi}^{\pi} \frac{dk_1 \cdots dk_d}{d - (\cos k_1 + \cos k_2 + \cdots + \cos k_d)}$$

↓ integrand só perto da origem.

$|\vec{k}| < \epsilon \ll 1$

$$\int \cdots \int \frac{dk_1 \cdots dk_d}{k_1^2 + k_2^2 + \cdots k_d^2} = \int_0^{\varepsilon} \frac{c\, k^{d-1}}{k^2}\, dk \quad ; \quad d \geq 3$$

$$= c \int_0^{\varepsilon} k^{d-3}\, dk$$

é FINITO para $\underline{\underline{d \geq 3}}$

$$R(n) = 1 - \frac{1}{\underbrace{G(n,n,t)}_{\text{Finito}}} \underline{<} 1 \quad \text{para } \underline{d \geq 3}$$

$\underline{\underline{3D}}$: a partícula pode nunca mais retornar à origem

$\hookrightarrow R = 1 - 0{,}65 \cdots q < 1 \rightarrow$ Se $\underline{q = 1}$:

$R = 0{,}3405 \ldots$