Markov Chain

$X_1, X_2, X_3, \cdots$ $\qquad X_j \in \{s_1, s_2, \cdots\}$

$$P_{ij} = P(X_n = s_j \mid X_{n-1} = s_i)$$

transition matrix

Defn. A Markov chain is called an ergodic chain if it is possible to go from every state to every state (not necessarily in one move)

Defn. A Markov chain is called a regular chain if some power of the transition matrix has only positive elements.

Clearly, regular $\Rightarrow$ ergodic but not the other way round.

The fundamental theorem about ergodic Markov chains is the existence of a stationary measure

$$w P = w \qquad w = (w_1, w_2, \dots, w_n)$$

$$w_i > 0$$

$$P^n \longrightarrow W = \begin{pmatrix} \leftarrow w \rightarrow \\ \vdots \\ \leftarrow w \rightarrow \end{pmatrix}$$

the interpretation of w_i

Mean recurrence time for state s_i is $\dfrac{1}{w_i}$

Examples

1. Ehrenfest chain (1907)

Imagine p molecules distributed in two container A and B

A B

The state of the system is the number of molecules in container A.

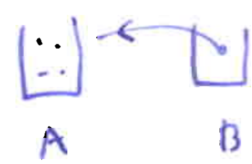
Thus the states are $\{0, 1, 2, \cdots, \rho\}$

$$k \to k-1, \qquad k \to k+1$$

At each stage a molecule is chosen and moved to the opposite container. The probability that a molecule in A is chosen if there are k molecules in container A is $\frac{k}{\rho}$; and hence, the prob. that a molecule in B is chosen is $\frac{\rho-k}{\rho}$.

Thus

$$p_{k,k+1} = \frac{\rho-k}{\rho} = 1 - \frac{k}{\rho}$$



$$p_{k,k-1} = \frac{k}{\rho}$$

Thus

$$\mathbb{P} = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ \vdots \\ \rho-1 \\ \rho \end{array} \begin{array}{c} \begin{array}{cccccc} 0 & 1 & 2 & 3 & \cdots & \rho \end{array} \\ \left[\begin{array}{cccccc} 0 & 1 & 0 & 0 & \cdots & 0 \\ 1/\rho & 0 & 1-\frac{1}{\rho} & 0 & \cdots & 0 \\ 0 & \frac{2}{\rho} & 0 & 1-\frac{2}{\rho} & \cdots & 0 \\ \vdots & & & & & \\ & & & & & \\ 0 & 0 & 0 & 0 & & \frac{1}{\rho} \\ 0 & 0 & 0 & 0 & 1 & 0 \end{array} \right] \end{array}$$

Find stationary measure

$$w\,\mathbb{P} = w \qquad\qquad w = (w_0, w_1, \cdots, w_\rho)$$

$$(w\mathbb{P})_k = \sum_{j=0}^{\rho} w_j\, P_{jk} = w_{k+1} P_{k+1,k} + w_{k-1} P_{k-1,k}$$

$$\mathbb{P}_{k,k+1} = 1 - \frac{k}{\rho} \qquad k \to k-1 \qquad P_{k-1,k} = 1 - \frac{k-1}{\rho}$$

$$\mathbb{P}_{k,k-1} = \frac{k}{\rho} \qquad k \to k+1 \qquad P_{k+1,k} = \frac{k+1}{\rho}$$

$$w_{k+1} \cdot \frac{k+1}{\rho} + \left(1 - \frac{k-1}{\rho}\right) w_{k-1} = w_k \qquad\qquad w_{-1} = 0$$

$$w_{\rho+1} = 0$$

then holds for $k = 0, 1, \cdots, \rho$.

Let $f(x) = \sum_{k=0}^{p} W_k x^k$

$$\frac{1}{p} \sum_{k=0}^{p} (k+1) W_{k+1} x^k + \sum_{k=0}^{p} W_{k-1} x^k$$

$$- \frac{1}{p} \sum_{k=0}^{p} (k-1) W_{k-1} x^k = \sum_{k=0}^{p} W_k x^k$$

$$\sum_{k=0}^{p} (k+1) W_{k+1} x^k = W_1 + 2W_2 x + \cdots + p W_p x^{p-1}$$

$$= f'(x)$$

$$\sum_{k=0}^{p} W_{k-1} x^k = W_0 x + W_1 x^2 + \cdots + W_{p-1} x^p$$

$$= x \left(W_0 + W_1 x + \cdots + W_{p-1} x^{p-1} \right)$$

$$= x \left(f(x) - W_p x^p \right)$$

$$\sum_{k=0}^{p} (k-1) W_{k-1} x^k = W_1 x^2 + 2 W_2 x^3 + \cdots + (p-1) W_{p-1} x^p$$

$$= x^2 \left(W_1 + 2W_2 x + \cdots + (p-1) W_{p-1} x^{p-2} \right)$$

$$\cancel{= x (f'(x))} = x^2 \left(f'(x) - p W_p x^{p-1} \right)$$

Thus

$$\frac{1}{p} f'(x) + x\left(f(x) - w_p x^p\right) - \frac{1}{p} x^2 \left(f'(x) - p w_p x^{p-1}\right) = f(x)$$

$$\frac{1}{p} f'(x) + x f(x) - \cancel{w_p x^{p+1}} - \frac{1}{p} x^2 f'(x) + \cancel{w_p x^{p+1}} = f(x)$$

$$\frac{1}{p}(1-x^2) f'(x) = (1-x) f(x)$$

$$\frac{1}{p}(1+x) f'(x) = f(x)$$

$$\frac{f'(x)}{f(x)} = \cancel{p\ell} \; \frac{p}{1+x}$$

$$\int \frac{f'}{f} dx = \int \frac{p}{1+x} dx$$

$$\log f = p \log(1+x) + C$$

$$f(x) = c(1+x)^p = c \sum_{k=0}^{p} \cancel{p} \binom{p}{k} x^k$$

$$\cancel{f(0)} \quad f(1) = \sum_{k=0}^{p} w_k = 1 \qquad f(1) = c\, 2^p = 1$$

$$c = 2^{-p}$$

$$f(x) = \sum_{k=0}^{p} \frac{1}{2^p} \binom{p}{k} x^k$$

Thus $\quad W_k = \frac{1}{2^\rho}\binom{\rho}{k}$ $\quad$ ρ = total # of molecules

k = # of molecules in container A

Physical Interpretation

Whatever the initial number of molecules in the first container, after a long time the probability of finding k molecules in it is nearly the same as if the ρ molecules had been distributed at random, each molecule having probability $1/2$ to be in the first container.

Let $D = \frac{k}{\rho}$ = density of gas in container A

Now $\quad k = \frac{1}{2}\rho + \sigma\sqrt{\rho}\, X$

k: random variable

X: random variable with $N(0,1)$

Thus

$$D = \frac{k}{\rho} = \frac{1}{2} + \frac{\sigma}{\sqrt{\rho}}\, X$$

Thermodynamics

– thus fluctuations about the mean are of order $\frac{1}{\sqrt{\rho}}$

— for $\rho \simeq 10^{23}$, fluctuations are very small.

Let $\rho = 2N$.

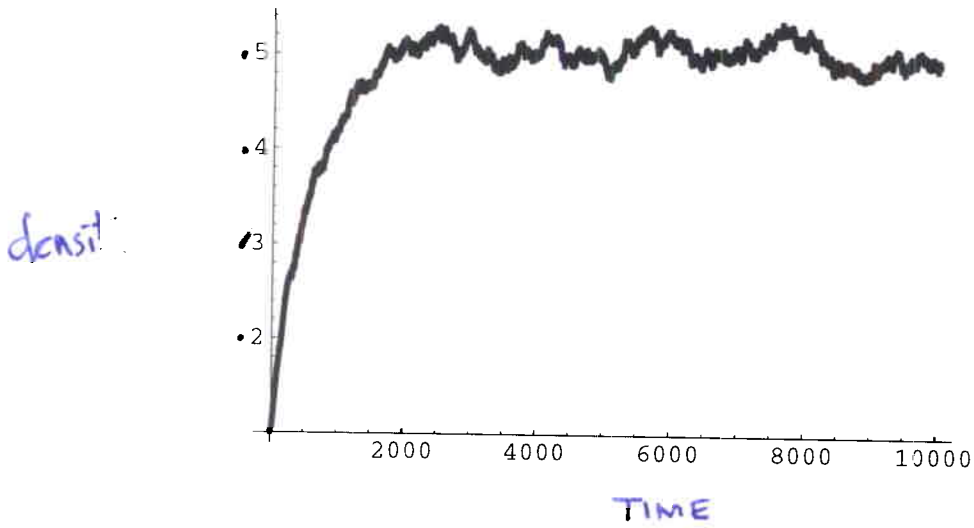
$$W_k = \frac{1}{2^{2N}} \binom{2N}{k}$$

Look at $W_N = \frac{1}{2^{2N}} \binom{2N}{N} \sim \frac{1}{\sqrt{\pi N}}$

Thus $r_N \sim \sqrt{\pi N}$ large recurrence times.

$$W_{N+k} \sim \frac{1}{\sqrt{\pi N}}\, e^{-\frac{1}{2} k/\sqrt{N}\sigma}$$

$$r_{N+k} \sim \sqrt{\pi N}\; e^{\frac{1}{2}\frac{k}{\sqrt{N}\sigma}}$$

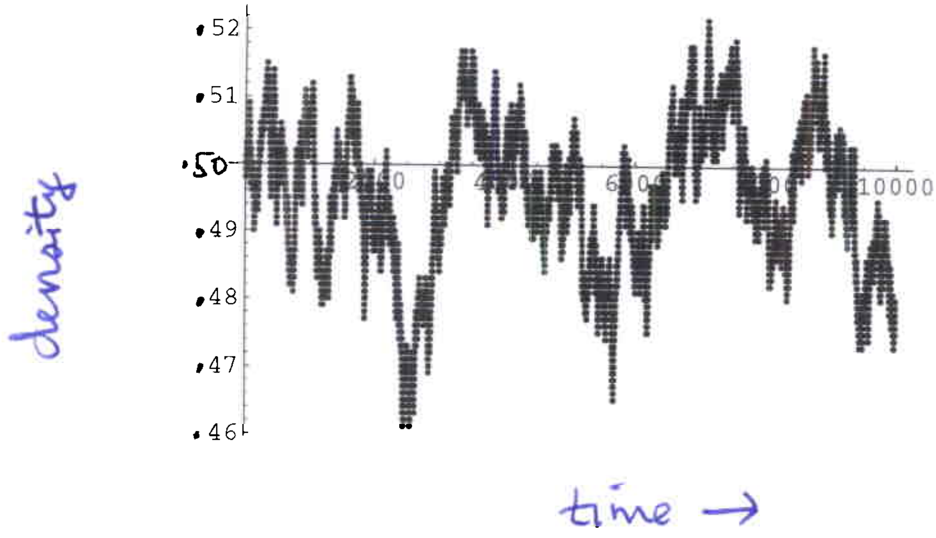


$n = 1000$ Molecules total
$k = 100$ Molecules in container A initially.

Above plot gives future k's as a function of time. I have divided k by n and plotted density.

We know that density $\rightarrow \frac{1}{2}$ for very large n. Here we can see approach to $\frac{1}{2}$ with the fluctuations around $\frac{1}{2}$.

Ran for 10,000 time steps



$n = 1000$ molecules

$k = 500$ molecules initially in container A.

Above plot shows the density fluctuations around the value ½. Note change of the density scale. We expect, roughly, fluctuations to be of order $\frac{1}{\sqrt{N}}$. Note

$$\frac{1}{\sqrt{1000}} \simeq 0.03$$

which is pretty good.

Simulation ran for 10,000 time steps.

Ergodic Theorem

$$w \underline{P} = w$$

Let $N_i(t)$ be the number of visits to the state i during times $0, 1, 2, \cdots, t-1$.

Then for any initial distribution

$$\frac{1}{t} N_i(t) \longrightarrow w_i \quad \text{as} \quad t \to \infty.$$

(this is a.s. convergence)

Two-State Markov Chain — Use of eigenvalues/eigenvectors

$$\mathbb{P} = \begin{pmatrix} 1-\alpha & \alpha \\ \beta & 1-\beta \end{pmatrix} \qquad 0 < \alpha, \beta < 1.$$

in this case we can compute $\mathbb{P}^n$ explicitly.

Eigenvalues are

$$1 \;,\; 1-\alpha-\beta$$

with corresponding eigenvectors

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \begin{pmatrix} -\alpha/\beta \\ 1 \end{pmatrix}$$

Thus

$$\mathbb{P} = \begin{pmatrix} 1 & -\alpha/\beta \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1-\alpha-\beta \end{pmatrix} \begin{pmatrix} 1 & -\alpha/\beta \\ 1 & 1 \end{pmatrix}^{-1}$$

thus

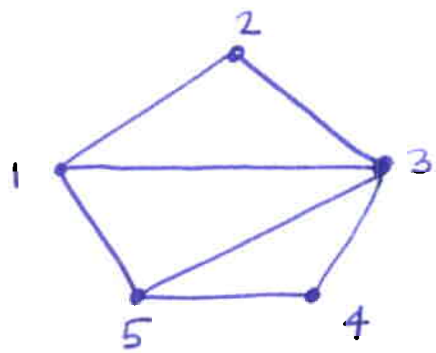
$$\mathbb{P}^n = \begin{pmatrix} 1 & -\alpha/\beta \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & (1-\alpha-\beta)^n \end{pmatrix} \begin{pmatrix} 1 & -\alpha/\beta \\ 1 & 1 \end{pmatrix}^{-1}$$

$c = (1-\alpha-\beta)^n$

$$\mathbb{P}^n = \begin{pmatrix} \dfrac{\beta+\alpha c}{\alpha+\beta} & \dfrac{\alpha-\alpha c}{\alpha+\beta} \\[2ex] \dfrac{\beta(z-1)}{\alpha+\beta} & \dfrac{\alpha+\beta z}{\alpha+\beta} \end{pmatrix}$$

Simple Random walk on a graph

$$\text{Graph} = (\underset{\substack{\uparrow \\ \text{edges}}}{E}, \overset{\substack{\text{vertices} \\ \downarrow}}{V})$$



We say vertices i and j are neighbors if there is an edge joining i and j

$\deg(i) = \#$ of neighbors of vertex i

State space = set of vertices

At each step the walker chooses one of its neighbors at random (uniform)

~~In ab~~
For above graph

$$P = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{bmatrix} 0 & 1/3 & 1/3 & 0 & 1/3 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 1/4 & 1/4 & 0 & 1/4 & 1/4 \\ 0 & 0 & 1/2 & 0 & \frac{1}{2} \\ 1/3 & 0 & 1/3 & 1/3 & 0 \end{bmatrix} \end{array}$$

More formally

$$P_{ij} = \begin{cases} \frac{1}{\deg(i)} & \text{if } i \text{ and } j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases}$$

Look at invariant measure

$$w P = w$$

<u>Proposition</u>

~~Let~~ Consider an ergodic Markov chain with state space S. Assume that there exists positive numbers w_i, $i \in S$ such that $\sum w_i = 1$ and

$$w_i P_{ij} = w_j P_{ji} \quad \text{for every } i,j \in S$$

Then $w = (w_1, w_2, \dots)$ is the equilibrium distr.

<u>Proof</u>

Must show $w P = w$

$$\sum_{i \in S} w_i P_{ij} = \sum_{i \in S} w_j P_{ji} = w_j \sum_i P_{ji} = w_j$$

since row sums $=1$.

Observe that if we can find positive numbers v_i such that

$$v_i P_{ij} = v_j P_{ji}$$

then can take

$$w_i = \frac{v_i}{\sum v_i}$$

This only assumes $\sum v_i < \infty$.

Return to simple random walk on Graph G

Claim $\quad w_i = \dfrac{\deg(i)}{Z} \qquad Z = \sum_{k \in S} \deg(k)$

Let $v_i = \deg(i)$

if i and j are not neighbors

$$v_i P_{ij} = 0 = v_j P_{ji} \quad \checkmark$$

if i and j are neighbors

$$v_i P_{ij} = \deg(i) \cdot \frac{1}{\deg(i)}$$

$$= 1 = \deg(j) \frac{1}{\deg(j)} = v_j P_{ji}$$

Thus

$$w = \left(\frac{3}{14}, \frac{2}{14}, \frac{4}{14}, \frac{2}{14}, \frac{3}{14} \right)$$ in above example

Defn.
A markov chain is called symmetric

if $\quad p_{ij} = p_{ji}$

Thus ~~if~~ $\quad w_i = \frac{1}{|S|}$ for all i