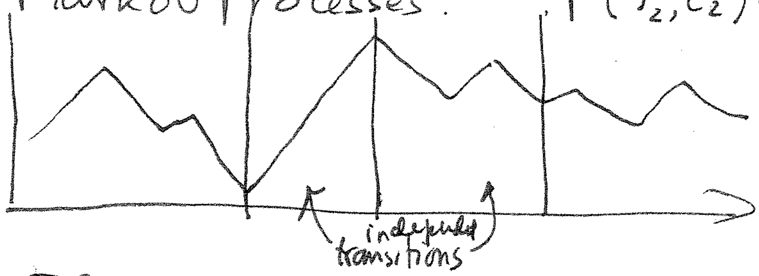
Stochastic Processes

Time dependent random variable examples.

Markov Processes: $P(y_2,t_2) = \int dy_1 \, P(y_2,t_2|y_1,t_1) P(y_1,$



If prob distr$\underset{..}{\text{n}}$ at future totally determined by the y at present.

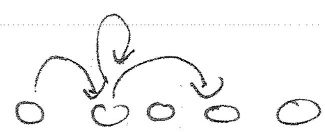
$t_1 < t_2 < t_3$ $\qquad P(y_3,t_3 | y_2,t_2 ; y_1,t_1) = P(y_3,t_3 | y_2,t$

Simplest example: Markov chain

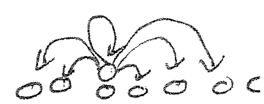
Y has M realizn. $\qquad y(1) \cdots y(M)$

$$P(n, s+1) = \sum_m Q_{nm}(s) \, P(m,s)$$

Q Transition matr.



Note that $\sum_n Q_{nm}(s) = 1$

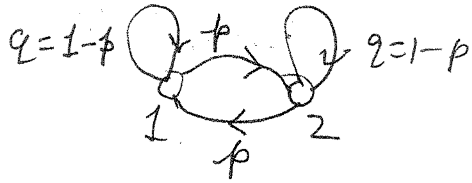


Example already seen: ~~[illegible]~~ Biased ranom walk

$$\begin{pmatrix} \ddots & & & & \\ & 0 & q & & \\ & p & 0 & q & \\ & & p & 0 & q \\ & & & p & 0 & \ddots \\ & & & & \ddots \end{pmatrix}$$

Matrix notation $\quad \mathbb{P}(s+1) = Q\,\mathbb{P}(s) \;\Rightarrow\; \mathbb{P}(s) = Q^s \mathbb{P}(0$

Let us take an even simpler example



$$Q = \begin{pmatrix} q & p \\ p & q \end{pmatrix}$$

Let us start with a state say $P(1) = 1 \quad P(2) = 0$

$$\mathbb{P}(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\mathbb{P}(s) = ? \qquad Q^s \, \mathbb{P}(0)$$

Note that Q has two eigenvectors $\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$

$$Q\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} p+q \\ p+q \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \Rightarrow \text{eigenvalue } \lambda_+ = 1$$

$$Q\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} q-p \\ p-q \end{pmatrix} = (q-p)\begin{pmatrix} 1 \\ -1 \end{pmatrix} \Rightarrow \text{eigenvalue } \lambda_- = q-p = 1-2p$$ [redacted]

Note that $|\lambda_-| < 1$

$$\mathbb{P}(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$Q^s \, \mathbb{P}(0) = \frac{Q^s}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{Q^s}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} + (1-2p)^s \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \end{pmatrix}$$

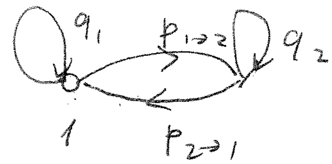
As $s \to \infty$ $\quad (1-2p)^s \to 0$, as long as $p \neq 0, 1$

So $\mathbb{P}(s) \to \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$ as $s \to \infty$

The convergence is determined by how small $|1-2p|$ is.

[redacted] Is $s \gg \frac{1}{\ln 1/|1-2p|}$ then $|1-2p|^s \ll 1$

[redacted] What if the system was assymetric ?



$$Q = \begin{pmatrix} q_1 & p_{2\to 1} \\ p_{1\to 2} & q_2 \end{pmatrix}$$

We could once more ask for the eigenvalues and eigenvectors. [redacted] We could do it by brute force. But let us do it [redacted] with less sweat

Note $\mathbb{1}^T Q = (1\ \ 1)\begin{pmatrix} q_1 & p_{2\to} \\ p_{1\to 2} & q_2 \end{pmatrix} = \left(q_1 + p_{1\to 2}\ \ q_2 + p_{2\to 1}\right) = \mathbb{1}^T$

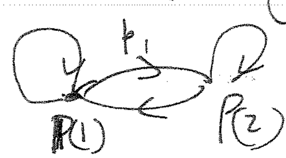
So [redacted] $\begin{pmatrix}1\\1\end{pmatrix}$ is [redacted] a left eigenvector as a consequence of prob conservn. The corresponding eigenvalue is 1

We know that the trace Q = sum of eigenvalues

$$1 + \lambda_- = q_1 + q_2 \Rightarrow \lambda_- = 1 - p_{1\to 2} - p_{2\to 1}\text{, Once more } |\lambda_-|$$

[redacted]

The right eigenvector corresponding to eigenvalue 1 is easy to figure out



$P(1)$ [redacted] would not change if loss $p_{1\to 2}P(1)$ equals gain $p_{2\to 1}P(2)$. So $\dfrac{P(1)}{P(2)} = \dfrac{p_{2\to 1}}{p_{1\to 2}} \Rightarrow P(1)\ \dfrac{P(1)}{P(1)+P(2)} = \dfrac{p_2}{p_{2}+p_{1\to 2}}$

$$\mathbb{P}(S) \rightarrow [redacted] \begin{pmatrix} \dfrac{p_{2\to 1}}{p_{2\to 1}+p_{1\to 2}} \\[2ex] \dfrac{p_{1\to 2}}{p_{2\to 1}+p_{1\to 2}} \end{pmatrix}$$

An example of detailed balance at work.

The timescale of convergence given by $1/\log\{1/(1-p_{1\to 2}-p_{2\to 1})\}$

That we always find one eigenvector with eigenvalue one is the consequence of probability conservation. The fact that all other eigenvalues turn out to be of smaller magnitude is the consequence of Perron Frobenius theorem

Def: Matrix is called positive (non-negative) means all entries are +ve (non-negative)

Often denoted as $A > 0$ $(A \geq 0)$

Def: A Matrix is called regular if $A^k > 0$ for $k \geq 1$

Perron-Frobenius Thm for regular matrices

For a non-negative regular matrix A

(a) There is an eigenvalue λ_{PF} of A that is real and positive with positive left and right eigenvectors (called the PF eigenvectors)

(b) For any other eigenvalue $|\lambda| < \lambda_{PF}$

(c) The eigenvalue λ_{PF} is simple, i.e. has multiplicity one and corresponds to 1×1 Jordan block.

If one drops the regularity condition and only has $A \geq 0$ λ_{PF} is real and nonneg with eigenvectors that are non negative

Other λ's are s.t. $|\lambda| \leq \lambda_{PF}$ (λ_{PF} need not be unique)

Irregular example  $Q = \begin{pmatrix} q & 0 \\ p & 1 \end{pmatrix}$

If we have a matrix like Q, which satisfies $Q \geq 0$ and $\mathbb{1}^T Q = \mathbb{1}^T$, Q is called a stochastic matrix.

Note that if v_{PF} is a right PF eigenvector then [redacted] [redacted] $Q v_{PF} = \lambda_{PF} v_{PF}$

But $(\mathbb{1}^T Q) v_{PF} = \mathbb{1}^T v_{PF}$

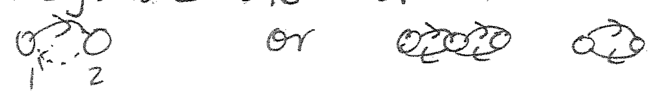
$\mathbb{1}^T (Q v_{PF}) = \lambda_{PF} \mathbb{1}^T v_{PF}$

Since $v_{PF} \neq 0$ and $v_{PF} \geq 0$ $\mathbb{1}^T v_{PF} \neq 0$

$\Rightarrow \boxed{\lambda_{PF} = 1}$

What does regularity [redacted] mean [redacted] in the context of stochastic processes? $Q^k_{ij} > 0$ means there is a nonzero probability of transition from j to i. Thus regularity [redacted] just means that if we take a [redacted] large enough [redacted] number of steps then every state to could be accessed from every other state in that. Note that for every pair i,j, there should be a path of the same length k.

Irregular stochastic matrices.



For simplicity we focus on the case where the [redacted] the right eigenvectors [redacted] each span the n dimensional vector space

Any $\mathbb{P}(0) = \sum \alpha_i u_i$ ← right eigenvector

$\mathbb{P}(s) = \sum \alpha_i Q^s u_i = \sum \alpha_i \lambda_i^s u_i$

$= \alpha_{PF} u_{PF} + \sum_{\lambda \neq \lambda_{PF}} \lambda_i^s u_i$

$|\lambda_i| < \lambda_{PF} = 1$ for regular Q

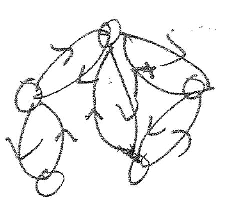
So finally $\mathbb{P}(s) \to \alpha_{PF} u_{PF} = \mathbb{P}_{ST}$
the stationary probability distribution.
If u_{PF} is normalized so that $\mathbb{1}^T u_{PF} = \sum_n u_{PF}(n) = 1$
then $\alpha_{PF} = 1$ $\quad u_{PF} = \mathbb{P}_{ST}$

Thus, if we have a finite number of states and have a regular transition matrix, we are guaranteed, in the long term to the stationary state. Also the stationary state is unique.

This observation could be utilized to do sampling from a probability distribution! Invent a stochastic process s.t. the stationary distr^n is the intended one. Let us invent a transition matrix Q s.t.

$Q_{nm} P(m) = Q_{mn} P(n)$

along with the condition that Q is regular.

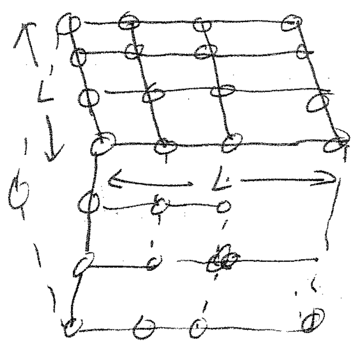


[Roughly meaning you could go from any state to any other state by these moves]

Why do you need this? If we know $P(n)$ why can't we just calculate $\sum_{m=1}^{M} O(m) P(m)$ for any average?

The answer is that often in Stat mech we are dealing with problems where M is exponential in the size of the system (or number of particles or spins -

Example: Particles on a lattice



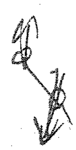
L^d sites

N particles $N \sim \rho L^d$

$(N)^{L^d}$ or ${}^{L^d}C_N$

depending upon hard core or not

Spins on a lattice $\sigma_i = \pm 1$



2^{L^d}

$L \sim 10^8 \left(= \frac{1\,cm}{1\,Å}\right)$

$L^2 \sim 10^{12}$ $L^3 \sim 10^{24}$ (close to Avogadro's #)

Even $2^{(10^8)}$ is huge!

~~Accepted~~ Allowed moves: Particle hopping. Spin flips -

Note that $\frac{Q_{nm}}{Q_{mn}} = \frac{P(n)}{P(m)}$ is satisfied by Q even if $Q_{nm} \to \lambda_{nm} Q_{nm}$ where λ_{nm} is symmetric. We need to make a choice!

One such choice leads to metropolis algorithm:

If $m \to n$ is an allowed move, take it with probability $\min(1, \frac{P(n)}{P(m)})$.

Convergence time is supposed to be finite, However as $N \to \infty$, it could tend to infinity.

Continuous time version of Markov Stochastic Process: Master equation

$$\frac{d}{dt} \mathbb{P}(t) = W \mathbb{P}(t)$$

$Q = \mathbb{1} + \Delta t W$

More explicitly $\frac{d}{dt} P(m,t) = \sum_n W_{mn} P(n,t)$

Note that $W_{mn} \geq 0$ for $m \neq n$, but $W_{nn} \leq 0$ so that $\sum_m W_{mn} = 0$

One could show that W always has a zero eigenvalue and, under appropriate conditions, all other eigenvalues have a neg. real part.