

### 5.D.3. Mean First Passage Time

For the random walk problem, the **mean first passage time** is the average time for the walker to reach some site  $n_p$  for the 1st time, assuming he started at site  $n_0$  at time  $t = 0$ . If we assume

$$P(n_p, t) \equiv 0 \quad \forall t \quad (a)$$

then the walker cannot return to the random walk once he reaches  $n_p$ . This is called an **absorbing boundary condition** at site  $n_p$ .

Since the walker is known to be at  $n_0$  at time  $t = 0$ , we can simplify the notations and set

$$Q_n(t) \equiv P_{1|1}(n_0, 0 | n, t) \quad (b)$$

$$\rightarrow Q_n(0) = P_{1|1}(n_0, 0 | n, 0) = \delta_{n, n_0} \quad (c)$$

Since

$$P(n, 0) = \begin{cases} 1 & n = n_0 \\ 0 & \text{otherwise} \end{cases}$$

we have

$$P(n, t) = P_{1|1}(n_0, 0 | n, t) = Q_n(t)$$

and (a) becomes

$$P(n_p, t) = P_{1|1}(n_0, 0 | n_p, t) = Q_{n_p}(t) = 0 \quad \forall t \quad (d)$$

The master equation (5.53) thus becomes

$$\frac{\partial Q_n(t)}{\partial t} = \sum_{m(\neq n_p)=1}^M Q_m(t) w_{mn}(t) - Q_n(t) \sum_{k=1}^M w_{nk}(t) \quad \forall n \neq n_p \quad (5.68)$$

Note that the  $m = n_p$  term was excluded in the 1st sum in order to enforce the condition  $Q_{n_p}(t) = 0$  [see (d)]. However, since  $w_{n n_p} \neq 0$  in general, it is still present in the 2nd sum.

In Dirac notations,

$$\frac{\partial \mathbf{Q}}{\partial t} = \mathbf{Q} \mathbf{M} \quad (5.69)$$

where

$$Q_n(t) = \langle n_0 | \mathbf{Q}(t) | n \rangle$$

$$\langle m | \mathbf{M} | n \rangle = \begin{cases} w_{mn} - \delta_{mn} \sum_{k=1}^M w_{nk} & m \text{ and } n \neq n_p \\ 0 & m \text{ or } n = n_p \end{cases} \quad (5.69e)$$

In order words,  $\mathbf{M}$  is just  $\mathbf{W}$  with the  $(n_p)^{\text{th}}$  row & column removed.

The probability that the walker is still alive ( i.e.,  $n \neq n_p$  ) at time  $t$  is

$$\mathcal{P}(t) \equiv \sum_{n(\neq n_p)=1}^M P(n, t) = \sum_{n(\neq n_p)=1}^M Q_n(t) \quad (5.70)$$

Let

$$f_{n_p}(t) dt \equiv \text{probability to reach site } n_p \text{ within time interval } (t, t + dt) \quad (5.71)$$

$$= \text{probability that the walker dies during } (t, t + dt)$$

Since the walker must either live or die at any instance, we have

$$\mathcal{P}(t) = f_{n_p}(t) dt + \mathcal{P}(t + dt) \quad (5.72)$$

$$\rightarrow \frac{d\mathcal{P}(t)}{dt} = \lim_{dt \rightarrow 0} \frac{\mathcal{P}(t + dt) - \mathcal{P}(t)}{dt} = -f_{n_p}(t) \quad (5.73)$$

Using (5.70) & (5.68), we can write (5.73) as

$$\begin{aligned}
 f_{n_p}(t) &= - \sum_{n(\neq n_p)=1}^M \frac{\partial Q_n(t)}{\partial t} \\
 &= - \sum_{n, m(\neq n_p)=1}^M Q_m(t) w_{mn}(t) + \sum_{n(\neq n_p)=1}^M Q_n(t) \sum_{k=1}^M w_{nk}(t) \\
 &= \sum_{n(\neq n_p)=1}^M Q_n(t) \left( - \sum_{k(\neq n_p)=1}^M w_{nk}(t) + \sum_{k=1}^M w_{nk}(t) \right) \\
 &= \sum_{n(\neq n_p)=1}^M Q_n(t) w_{nn_p}(t)
 \end{aligned} \tag{5.74}$$

Note that  $f_{n_p}(t)$ ,  $Q_n(t)$  and  $w_{nn_p}(t)$  are all real & positive.

The mean first passage time is therefore

$$\begin{aligned}
 \langle t \rangle &= \int_0^\infty dt f_{n_p}(t) t && (5.75) \\
 &= - \int_0^\infty t d\mathcal{P}(t) && [(5.72) \text{ used.}] \\
 &= -t\mathcal{P}(t) \Big|_0^\infty + \int_0^\infty dt \mathcal{P}(t) \\
 &= \int_0^\infty dt \mathcal{P}(t) && (5.75a)
 \end{aligned}$$

where we've assumed the the walker dies at some finite time  $T$  so that

$$\begin{aligned}
 \mathcal{P}(t) &= 0 && \forall t \geq T \\
 \rightarrow \lim_{t \rightarrow \infty} t\mathcal{P}(t) &= 0
 \end{aligned}$$

### Exercise 5.4

Consider an asymmetric random walk on a lattice with 5 lattice sites. Assume the 5<sup>th</sup> site,  $P$ , absorbs the walker. The transition rates are

$$\begin{aligned}
 w_{1,2} = w_{1,3} = w_{1,4} = w_{1,P} &= \frac{1}{4} && w_{2,1} = w_{2,3} = w_{2,P} = \frac{1}{3} \\
 w_{3,1} = w_{3,2} = w_{3,4} &= \frac{1}{3} && w_{4,1} = w_{4,3} = w_{4,P} = \frac{1}{3} \\
 w_{P,1} = w_{P,2} = w_{P,4} &= \frac{1}{3}
 \end{aligned}$$

and  $w_{ij} = 0$  otherwise.

- (a) Write the transition matrix  $M$  and find its eigenvalues and left & right eigenvectors.
- (b) If the walker starts at site  $n = 3$  at time  $t = 0$ , compute the mean first passage time.

### Answer (a)

With  $P = 5$ , the transition matrix is

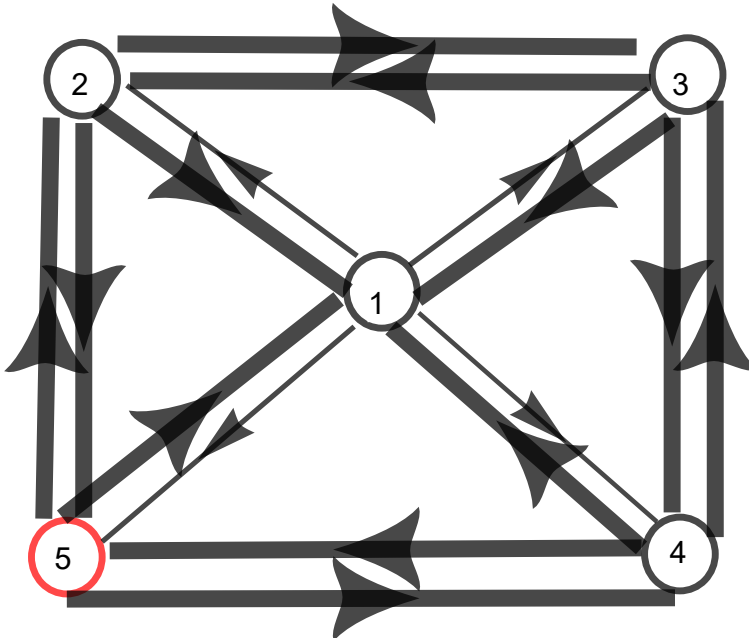
$$W = \begin{pmatrix} -1 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{3} & -1 & \frac{1}{3} & 0 & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & -1 & \frac{1}{3} & 0 \\ \frac{1}{3} & 0 & \frac{1}{3} & -1 & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} & -1 \end{pmatrix}$$

$$\rightarrow M = \begin{pmatrix} -1 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{3} & -1 & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & -1 & \frac{1}{3} \\ \frac{1}{3} & 0 & \frac{1}{3} & -1 \end{pmatrix}$$

Connection graph for  $W$ . Thick arrows have strength  $\frac{1}{3}$ , thin ones  $\frac{1}{4}$ .

Number of arrows going out site  $n$  = number of non-zero off-diagonal entries in row  $n$ .

Number of arrows going into site  $n$  = number of non-zero off-diagonal entries in column  $n$ .



The eigenvalues and eigenvectors of  $M$  are [ see §Code (a) ]

$$\lambda_1 = -1.5 \quad \lambda_2 = -1.28359 \quad \lambda_3 = -1.0 \quad \lambda_4 = -0.216406$$

$$| \chi_1^R \rangle = \begin{pmatrix} -0.5 \\ 1.0 \\ -1.0 \\ 1.0 \end{pmatrix} \quad | \chi_2^R \rangle = \begin{pmatrix} -8.55234 \\ 1.0 \\ 7.70156 \\ 1.0 \end{pmatrix} \quad | \chi_3^R \rangle = \begin{pmatrix} 0 \\ -1.0 \\ 0 \\ 1.0 \end{pmatrix} \quad | \chi_4^R \rangle = \begin{pmatrix} 1.05234 \\ 1.0 \\ 1.29844 \\ 1.0 \end{pmatrix}$$

$$\langle \chi_1^L | = (-0.666667, 1, -1, 1) \quad \langle \chi_2^L | = (-11.4031, 1, 7.70156, 1)$$

$$\langle \chi_3^L | = (0, -1, 0, 1) \quad \langle \chi_4^L | = (1.40312, 1., 1.29844, 1.)$$

As usual, we normalize by leaving  $| \chi_i^R \rangle$  alone and set

$$\langle \chi_i^L | \rightarrow \frac{\langle \chi_i^L |}{\langle \chi_i^L | \chi_i^R \rangle}$$

so that

$$\langle \chi_1^L | = (-0.2, 0.3, -0.3, 0.3)$$

$$\langle \chi_3^L | = (0, -0.5, 0, 0.5)$$

$$\langle \chi_2^L | = (-0.0718, 0.00630, 0.0485, 0.00630)$$

$$\langle \chi_4^L | = (0.272, 0.194, 0.252, 0.194)$$

See §Code (a) for proof that these eigenvectors are orthonormal & complete.

### Code (a)

$$\text{In[1]:= } \mathbf{M} = \begin{pmatrix} -1 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{3} & -1 & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & -1 & \frac{1}{3} \\ \frac{1}{3} & 0 & \frac{1}{3} & -1 \end{pmatrix};$$

In[2]:= **(\* Eigenvalues & right eigenvectors \*)**  
 $\{\lambda, \text{rev}\} = \text{Eigensystem}[\mathbf{M}]$

$$\text{Out[2]:= } \left\{ \left\{ -\frac{3}{2}, \frac{1}{12} (-9 - \sqrt{41}), -1, \frac{1}{12} (-9 + \sqrt{41}) \right\}, \right. \\ \left. \left\{ -\frac{1}{2}, 1, -1, 1 \right\}, \left\{ \frac{3(-31 + 5\sqrt{41})}{2(-45 + 7\sqrt{41})}, 1, -\frac{59 - 9\sqrt{41}}{-45 + 7\sqrt{41}}, 1 \right\}, \right. \\ \left. \left\{ 0, -1, 0, 1 \right\}, \left\{ \frac{3(31 + 5\sqrt{41})}{2(45 + 7\sqrt{41})}, 1, -\frac{-59 - 9\sqrt{41}}{45 + 7\sqrt{41}}, 1 \right\} \right\}$$

In[3]:= **(\* Numerical values \*)**  
 $\{\lambda, \text{rev}\} // \mathbf{N}$

$$\text{Out[3]:= } \left\{ \{-1.5, -1.28359, -1., -0.216406\}, \{-0.5, 1., -1., 1.\}, \right. \\ \left. \{-8.55234, 1., 7.70156, 1.\}, \{0., -1., 0., 1.\}, \{1.05234, 1., 1.29844, 1.\} \right\}$$

In[4]:= **(\* Eigenvalues & left eigenvectors \*)**  
 $\{\lambda, \text{lev}\} = \text{Eigensystem}[\mathbf{M}^T]$

$$\text{Out[4]:= } \left\{ \left\{ -\frac{3}{2}, \frac{1}{12} (-9 - \sqrt{41}), -1, \frac{1}{12} (-9 + \sqrt{41}) \right\}, \right. \\ \left. \left\{ -\frac{2}{3}, 1, -1, 1 \right\}, \left\{ \frac{2(-31 + 5\sqrt{41})}{-45 + 7\sqrt{41}}, 1, -\frac{59 - 9\sqrt{41}}{-45 + 7\sqrt{41}}, 1 \right\}, \right. \\ \left. \left\{ 0, -1, 0, 1 \right\}, \left\{ \frac{2(31 + 5\sqrt{41})}{45 + 7\sqrt{41}}, 1, -\frac{-59 - 9\sqrt{41}}{45 + 7\sqrt{41}}, 1 \right\} \right\}$$

In[5]:= **(\* Numerical values \*)**  
 $\{\lambda, \text{lev}\} // \mathbf{N}$

$$\text{Out[5]:= } \left\{ \{-1.5, -1.28359, -1., -0.216406\}, \{-0.666667, 1., -1., 1.\}, \right. \\ \left. \{-11.4031, 1., 7.70156, 1.\}, \{0., -1., 0., 1.\}, \{1.40312, 1., 1.29844, 1.\} \right\}$$

In[16]:=  $\text{levn} = \text{Table}\left[\frac{\text{lev}[[i]]}{\text{lev}[[i]].\text{rev}[[i]]}, \{i, 4\}\right];$   
 $\text{levn} // \mathbf{N}[\#, 3] \&$

$$\text{Out[17]:= } \left\{ \{-0.200, 0.300, -0.300, 0.300\}, \{-0.0718, 0.00630, 0.0485, 0.00630\}, \right. \\ \left. \{0, -0.500, 0, 0.500\}, \{0.272, 0.194, 0.252, 0.194\} \right\}$$

In[8]:= (\* orthonormality \*)

Table[ levn[[i].rev[[j]], {i, 4}, {j, 4}] // N // MatrixForm

Out[8]//MatrixForm=

$$\begin{pmatrix} 1. & 4.44089 \times 10^{-16} & 0. & -2.77556 \times 10^{-17} \\ 6.93889 \times 10^{-18} & 1. & 0. & 1.94289 \times 10^{-16} \\ 0. & 0. & 1. & 0. \\ 0. & 6.21725 \times 10^{-15} & 0. & 1. \end{pmatrix}$$

In[9]:= % // Chop // MatrixForm

Out[9]//MatrixForm=

$$\begin{pmatrix} 1. & 0 & 0 & 0 \\ 0 & 1. & 0 & 0 \\ 0 & 0 & 1. & 0 \\ 0 & 0 & 0 & 1. \end{pmatrix}$$

In[10]:= (\*  $|\chi_i^R\rangle\langle\chi_i^L|$  \*)

r1Prod = Table[Outer[Times, rev[[i], levn[[i]]], {i, 4}] // N;  
MatrixForm/@r1Prod

$$\text{Out[11]= } \left\{ \begin{pmatrix} 0.1 & -0.15 & 0.15 & -0.15 \\ -0.2 & 0.3 & -0.3 & 0.3 \\ 0.2 & -0.3 & 0.3 & -0.3 \\ -0.2 & 0.3 & -0.3 & 0.3 \end{pmatrix}, \begin{pmatrix} 0.613982 & -0.0538434 & -0.414678 & -0.0538434 \\ -0.0717911 & 0.00629574 & 0.0484871 & 0.00629574 \\ -0.552904 & 0.0484871 & 0.373426 & 0.0484871 \\ -0.0717911 & 0.00629574 & 0.0484871 & 0.00629574 \end{pmatrix}, \right.$$

$$\left. \begin{pmatrix} 0. & 0. & 0. & 0. \\ 0. & 0.5 & 0. & -0.5 \\ 0. & 0. & 0. & 0. \\ 0. & -0.5 & 0. & 0.5 \end{pmatrix}, \begin{pmatrix} 0.286018 & 0.203843 & 0.264678 & 0.203843 \\ 0.271791 & 0.193704 & 0.251513 & 0.193704 \\ 0.352904 & 0.251513 & 0.326574 & 0.251513 \\ 0.271791 & 0.193704 & 0.251513 & 0.193704 \end{pmatrix} \right\}$$

In[12]:= (\* Completeness:  $\sum_{i=1}^4 |\psi_i\rangle\langle\chi_i| = \mathbf{I}$  \*)

$\sum_{i=1}^4$  r1Prod[[i]] // MatrixForm

Out[12]//MatrixForm=

$$\begin{pmatrix} 1. & -2.77556 \times 10^{-16} & -5.55112 \times 10^{-17} & -2.77556 \times 10^{-16} \\ -3.88578 \times 10^{-16} & 1. & 3.33067 \times 10^{-16} & 5.55112 \times 10^{-17} \\ -1.66533 \times 10^{-16} & 3.33067 \times 10^{-16} & 1. & 3.33067 \times 10^{-16} \\ -3.88578 \times 10^{-16} & 5.55112 \times 10^{-17} & 3.33067 \times 10^{-16} & 1. \end{pmatrix}$$

In[13]:= % // Chop // MatrixForm

Out[13]//MatrixForm=

$$\begin{pmatrix} 1. & 0 & 0 & 0 \\ 0 & 1. & 0 & 0 \\ 0 & 0 & 1. & 0 \\ 0 & 0 & 0 & 1. \end{pmatrix}$$

## Answer (b)

Since  $M$  is time independent, (5.69) gives

$$\begin{aligned} \mathbf{Q}(t) &= \mathbf{Q}(0) e^{Mt} \\ &= \mathbf{Q}(0) \sum_{i=1}^4 |\chi_i^R\rangle e^{\lambda_i t} \langle\chi_i^L| \end{aligned} \quad (1)$$

Using

$$\langle n_0 | \mathbf{Q}(0) | m \rangle = \delta_{n_0 m}$$

we have

$$Q_n(t) \equiv \langle n_0 | \mathbf{Q}(t) | n \rangle$$

$$\begin{aligned}
&= \sum_{m=1}^4 \langle n_0 \mid \mathbf{Q}(0) \mid m \rangle \sum_{i=1}^4 \langle m \mid \chi_i^R \rangle e^{\lambda_i t} \langle \chi_i^L \mid n \rangle \\
&= \sum_{i=1}^4 \langle n_0 \mid \chi_i^R \rangle e^{\lambda_i t} \langle \chi_i^L \mid n \rangle
\end{aligned} \tag{2}$$

(5.70) thus becomes

$$\begin{aligned}
\mathcal{P}(t) &= \sum_{n=1}^4 Q_n(t) \\
&= \sum_{n=1}^4 \sum_{i=1}^4 \langle n_0 \mid \chi_i^R \rangle e^{\lambda_i t} \langle \chi_i^L \mid n \rangle
\end{aligned}$$

(5.75) then gives the mean first passage time as

$$\begin{aligned}
\langle t \rangle &= \int_0^\infty dt \mathcal{P}(t) \\
&= \sum_{n=1}^4 \sum_{i=1}^4 \langle n_0 \mid \chi_i^R \rangle \int_0^\infty dt e^{\lambda_i t} \langle \chi_i^L \mid n \rangle \\
&= \sum_{n=1}^4 \sum_{i=1}^4 \langle n_0 \mid \chi_i^R \rangle \left( -\frac{1}{\lambda_i} \right) \langle \chi_i^L \mid n \rangle \\
&= - \sum_{n=1}^4 \sum_{i=1}^4 \frac{1}{\lambda_i} \chi_i^R(n_0) \chi_i^L(n)
\end{aligned} \tag{3}$$

For  $n_0 = 3$ , we have  $\langle t \rangle \approx 5.333$  [ see §Code (b) ].

### Code (b)

```

(* mean 1st passage time *)
m1pt[n0_] := - Sum[Sum[1/lambda[[i]], {i, 1, 4}], {n, 1, 4}] rev[[i, n0]] levn[[i, n]]

(* n0=3 *)
m1pt[3] // N
5.33333

```