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

$$P(n_p, t) \equiv 0 \qquad \forall\ t \tag{a}$$

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

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

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

Since

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

we have

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

and (a) becomes

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

The master equation (5.53) thus becomes

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

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,

$$\frac{\partial\, \boldsymbol{Q}}{\partial\, t} = \boldsymbol{Q}\,\boldsymbol{M} \tag{5.69}$$

where

$$Q_n(t) = \langle n_0 \mid \boldsymbol{Q}(t) \mid n \rangle$$

$$\langle m \mid \boldsymbol{M} \mid n \rangle = \begin{cases} w_{m\,n} - \delta_{m\,n} \sum_{k=1}^{M} w_{n\,k} & m \text{ and } n \neq n_p \\ 0 & m \text{ or } n = n_p \end{cases} \tag{5.69e}$$

In order words, $\boldsymbol{M}$ is just $\boldsymbol{W}$ 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

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

Let

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

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

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

$$\mathcal{P}(t) = f_{n_p}(t)\, d\,t + \mathcal{P}(t + d\,t) \tag{5.72}$$

$$\rightarrow \qquad \frac{d\,\mathcal{P}(t)}{d\,t} = \lim_{d\,t \to 0} \frac{\mathcal{P}(t + d\,t) - \mathcal{P}(t)}{d\,t} = -f_{n_p}(t) \tag{5.73}$$

Using (5.70) & (5.68), we have

$$f_{n_p}(t) = -\sum_{n(\neq n_p)=1}^{M} \frac{\partial Q_n(t)}{\partial t}$$

$$= -\sum_{n,m(\neq n_p)=1}^{M} Q_m(t)\, w_{mn}(t) + \sum_{n(\neq n_p)=1}^{M} Q_n(t) \sum_{k=1}^{M} w_{nk}(t)$$

$$= \sum_{n(\neq n_p)=1}^{M} Q_n(t) \left(-\sum_{k(\neq n_p)=1}^{M} w_{nk}(t) + \sum_{k=1}^{M} w_{nk}(t) \right)$$

$$= \sum_{n(\neq n_p)=1}^{M} Q_n(t)\; w_{n n_p}(t) \qquad (5.74)$$

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

The mean first passage time is therefore

$$\langle t \rangle = \int_0^\infty d t\, f_{n_p}(t)\, t \qquad (5.75)$$

$$= -\int_0^\infty t\, d\mathcal{P}(t) \qquad \text{[(5.72) used.]}$$

$$= -t\,\mathcal{P}(t)\Big|_0^\infty + \int_0^\infty d t\; \mathcal{P}(t)$$

$$= \int_0^\infty d t\; \mathcal{P}(t) \qquad (5.75a)$$

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

$$\mathcal{P}(t) = 0 \qquad \forall\; t \geq T$$

$$\to \qquad \lim_{t\to\infty} t\,\mathcal{P}(t) = 0$$

Exercise 5.4

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

$$w_{1,2} = w_{1,3} = w_{1,4} = w_{1,P} = \frac{1}{4} \qquad w_{2,1} = w_{2,3} = w_{2,P} = \frac{1}{3}$$

$$w_{3,1} = w_{3,2} = w_{3,4} = \frac{1}{3} \qquad w_{4,1} = w_{4,3} = w_{4,P} = \frac{1}{3}$$

$$w_{P,1} = w_{P,2} = w_{P,4} = \frac{1}{3}$$

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)

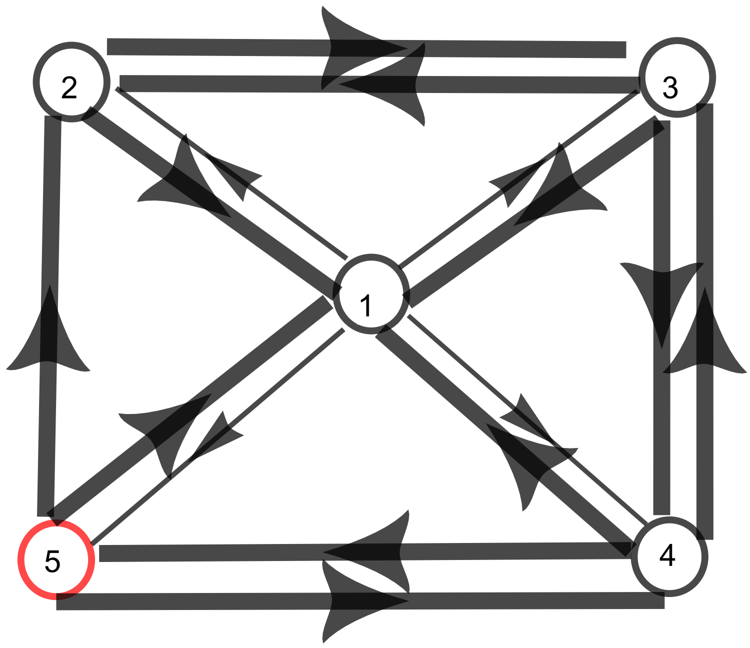
With $P = 5$, the transition matrix is

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

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

Connection graph for $\boldsymbol{W}$. 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 $\boldsymbol{M}$ are [see §Code (a)]

$\lambda_1 = -1.5$ $\qquad \lambda_2 = -1.28359$ $\qquad \lambda_3 = -1.0$ $\qquad \lambda_1 = -0.216406$

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

$\left\langle \chi_1^L \right| = (-0.666667,\ 1.0,\ -1.0,\ 1.0)$ $\left\langle \chi_2^L \right| = (-11.4031,\ 1.0,\ 7.70156,\ 1.0)$

$\left\langle \chi_3^L \right| = (0.,\ -1.0,\ 0.,\ 1.0)$ $\qquad \left\langle \chi_4^L \right| = (1.40312,\ 1.0,\ 1.29844,\ 1.0)$

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

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

so that

$\langle \chi_1^L | = (-0.2, 0.3, -0.3, 0.3)$ $\langle \chi_2^L | = (-0.0718, 0.00630, 0.0485, 0.00630)$
$\langle \chi_3^L | = (0, -0.5, 0, 0.5)$ $\langle \chi_4^L | = (0.272, 0.194, 0.252, 0.194)$

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

Code (a)

In[2]:=
$$M = \begin{pmatrix} -1 & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{3} & -1 & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & -1 & \frac{1}{3} \\ \frac{1}{3} & 0 & \frac{1}{3} & -1 \end{pmatrix};$$

In[3]:=
```
(* Eigenvalues & right eigenvectors *)
{λ, rev} = Eigensystem[M]
```

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

In[4]:=
```
(* Numerical values *)
{λ, rev} // N
```

Out[4]=
```
{{-1.5, -1.28359, -1., -0.216406}, {{-0.5, 1., -1., 1.},
  {-8.55234, 1., 7.70156, 1.}, {0., -1., 0., 1.}, {1.05234, 1., 1.29844, 1.}}}
```

In[5]:=
```
(* Eigenvalues & left eigenvectors *)
{λ, lev} = Eigensystem[Mᵀ]
```

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

In[14]:=
```
(* Numerical values *)
{λ, lev} // N[#, 3] &
```

Out[14]=
```
{{-1.50, -1.28, -1.00, -0.216}, {{-0.667, 1.00, -1.00, 1.00},
  {-11.4, 1.00, 7.70, 1.00}, {0, -1.00, 0, 1.00}, {1.40, 1.00, 1.30, 1.00}}}
```

In[12]:=
$$\text{levn} = \text{Table}\left[\frac{\text{lev}[[i]]}{\text{lev}[[i]].\text{rev}[[i]]}, \{i, 4\}\right];$$
```
levn // N[#, 3] &
```

Out[13]=
```
{{-0.200, 0.300, -0.300, 0.300}, {-0.0718, 0.00630, 0.0485, 0.00630},
 {0, -0.500, 0, 0.500}, {0.272, 0.194, 0.252, 0.194}}
```

In[35]:=
```
(* orthonormality *)
Table[ levn[[i]].rev[[j]], {i, 4}, {j, 4}] // N // MatrixForm
```

Out[35]//MatrixForm=

$$\begin{pmatrix} 1. & 4.44089\times10^{-16} & 0. & -2.77556\times10^{-17} \\ 6.93889\times10^{-18} & 1. & 0. & 1.94289\times10^{-16} \\ 0. & 0. & 1. & 0. \\ 0. & 6.21725\times10^{-15} & 0. & 1. \end{pmatrix}$$

In[36]:=
```
% // Chop // MatrixForm
```

Out[36]//MatrixForm=

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

In[20]:= (* $|\chi_i^R\rangle\langle\chi_i^L|$ *)
```
rlProd = Table[Outer[Times, rev[[i]], levn[[i]]], {i, 4}] // N;
MatrixForm /@ rlProd
```

Out[21]=

$$\left\{ \begin{pmatrix} 0.1 & -0.15 & 0.15 & -0.15 \\ -0.2 & 0.3 & -0.3 & 0.3 \\ 0.2 & -0.3 & 0.3 & -0.3 \\ -0.2 & 0.3 & -0.3 & 0.3 \end{pmatrix}, \begin{pmatrix} 0.613982 & -0.0538434 & -0.414678 & -0.0538434 \\ -0.0717911 & 0.00629574 & 0.0484871 & 0.00629574 \\ -0.552904 & 0.0484871 & 0.373426 & 0.0484871 \\ -0.0717911 & 0.00629574 & 0.0484871 & 0.00629574 \end{pmatrix}, \begin{pmatrix} 0. & 0. & 0. & 0. \\ 0. & 0.5 & 0. & -0.5 \\ 0. & 0. & 0. & 0. \\ 0. & -0.5 & 0. & 0.5 \end{pmatrix}, \begin{pmatrix} 0.286018 & 0.203843 & 0.264678 & 0.203843 \\ 0.271791 & 0.193704 & 0.251513 & 0.193704 \\ 0.352904 & 0.251513 & 0.326574 & 0.251513 \\ 0.271791 & 0.193704 & 0.251513 & 0.193704 \end{pmatrix} \right\}$$

In[32]:= (* Completeness: $\sum_{i=1}^{3} |\psi_i\rangle\langle\chi_i| = I$ *)

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

Out[32]//MatrixForm=

$$\begin{pmatrix} 1. & -2.77556\times10^{-16} & -5.55112\times10^{-17} & -2.77556\times10^{-16} \\ -3.88578\times10^{-16} & 1. & 3.33067\times10^{-16} & 5.55112\times10^{-17} \\ -1.66533\times10^{-16} & 3.33067\times10^{-16} & 1. & 3.33067\times10^{-16} \\ -3.88578\times10^{-16} & 5.55112\times10^{-17} & 3.33067\times10^{-16} & 1. \end{pmatrix}$$

In[34]:=
```
% // Chop // MatrixForm
```

Out[34]//MatrixForm=

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

Answer (b)

Since $\boldsymbol{M}$ is time independent, (5.69) gives

$$\boldsymbol{Q}(t) = \boldsymbol{Q}(0)\, e^{\boldsymbol{M}t}$$

$$= \boldsymbol{Q}(0) \sum_{i=1}^{4} |\chi_i^R\rangle e^{\lambda_i t} \langle \chi_i^L|$$

Using

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

we have

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

$$= \sum_{m=1}^{4} \langle n_0 \mid \boldsymbol{Q}(0) \mid m \rangle \sum_{i=1}^{4} \langle m \mid \chi_i^R \rangle e^{\lambda_i t} \langle \chi_i^L \mid n \rangle$$

$$= \sum_{i=1}^{4} \langle n_0 \mid \chi_i^R \rangle e^{\lambda_i t} \langle \chi_i^L \mid n \rangle$$

(5.70) thus becomes

$$\mathcal{P}(t) = \sum_{n=1}^{4} Q_n(t)$$

$$= \sum_{n=1}^{4} \sum_{i=1}^{4} \langle n_0 \mid \chi_i^R \rangle e^{\lambda_i t} \langle \chi_i^L \mid n \rangle$$

(5.75) then gives the mean first passage time as

$$\langle t \rangle = \int_0^\infty d\, t\, \mathcal{P}(t)$$

$$= \sum_{n=1}^{4} \sum_{i=1}^{4} \langle n_0 \mid \chi_i^R \rangle \int_0^\infty d\, t\, e^{\lambda_i t} \langle \chi_i^L \mid n \rangle$$

$$= \sum_{n=1}^{4} \sum_{i=1}^{4} \langle n_0 \mid \chi_i^R \rangle \left(-\frac{1}{\lambda_i} \right) \langle \chi_i^L \mid n \rangle$$

$$= -\sum_{n=1}^{4} \sum_{i=1}^{4} \frac{1}{\lambda_i} \chi_i^R (n_0)\, \chi_i^L (n)$$

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/λ[[i]] rev[[i, n0]] levn[[i, n]], {i, 1, 4}], {n, 1, 4}]

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

Out[30]= 5.33333