Chapter 16

Reversibility and detailed balance

Suppose a stochastic process evolves according to a Markov chain. For example a sequence of coin tosses:

$$\cdots \mathsf{HTTHTTTHTHH} \cdots \qquad .$$

In a long sequence, for an irreducible chain, we know there is a repeated pattern that emerges. Although this pattern is random, it is predictable to the extent that the law of large numbers hold. So given the future repeats the past, would we be able to tell if the sequence was forwards in time or backwards in time? That is, if the sequence has settled into a state of equilibrium can we distinguish the arrow of time ?

16.1 Detailed balance

Consider a Markov chain long into the sequence. Then one could assign a forward sequence and backward sequence by the labelling: $Y_n = X_{1-n}$. So an ascending index for Y (forward in the chain for Y) corresponds to a descending index for X (running backwards in time, or *in reverse*).

$$\begin{gathered} \ldots X_{-2}\ X_{-1}\ X_0\ X_1\ X_2\ \ldots \rightarrow \text{forwards} \\ \ldots Y_3\ Y_2\ Y_1\ Y_0\ Y_{-1}\ \ldots \leftarrow \text{backward.} \end{gathered}$$

As before, for the Markov chain, we have the transition matrix:

$$P(X_1 = k | X_0 = j) = p_{jk} \qquad . \tag{16.1}$$

Consider a transition in reverse:

$$\begin{aligned} P(Y_1 = k | Y_0 = j) &= \frac{P(Y_1 = k \text{ and } Y_0 = j)}{P(Y_0 = j)} \\ &= \frac{P(X_0 = k \text{ and } X_1 = j)}{P(Y_0 = j)} \\ &= \frac{P(X_0 = k \text{ and } X_1 = j)}{P(X_0 = j)} \times \frac{P(Y_1 = k)}{P(Y_0 = j)}. \end{aligned}$$

Then it follows that:

$$\frac{P(X_0 = k \text{ and } X_1 = j)}{P(X_0 = j)} = P(X_1 = j | X_0 = k) = p_{kj} \qquad . \tag{16.2}$$

However for a homogeneous chain this must be true at all points in the chain. For a *stationary* state the probability of any state (by the law of large numbers) is given by the equilibrium distribution, therefore:

$$\boxed{\frac{P(Y_1 = k)}{P(Y_0 = j)} = \frac{\pi_k}{\pi_j}} \qquad . \tag{16.3}$$

Therefore:

$$P(Y_1 = k | Y_0 = j) = \frac{\pi_k}{\pi_j} p_{kj} \qquad . \tag{16.4}$$

Now suppose that the chain is *reversible*. In mathematical terms we mean that the transition matrix going backwards is the same as that going forwards:

$$P(Y_1 = k | Y_0 = j) = p_{jk} \tag{16.5}$$

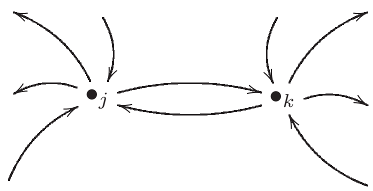
Then it follows, from equation (16.4), that:

$$p_{jk} = \frac{\pi_k}{\pi_j} p_{kj} \qquad . \tag{16.6}$$

This can be written in the symmetric form, the *detailed balance* equation:

$$\boxed{\pi_j p_{jk} = \pi_k p_{kj}} \qquad . \tag{16.7}$$

A reversible irreducible chain in equilibrium satisfies the equation of *detailed balance*. This equation can be understood in terms of the equilibrium of probability flow.



$$\begin{aligned} \pi_j p_{jk} &= \text{ flow of probability from } j \text{ to } k \\ \pi_j &= \text{ amount of probability at } j \\ p_{jk} &= \text{ transition rate out of } j \text{ into } k \\ \pi_k p_{kj} &= \text{ flow of probability from } k \text{ to } j. \end{aligned}$$

Detailed balance means that *every* pair of states is in equilibrium (microreversibility).

EXAMPLE Sainsburys/Tesco

A single customer jumps between these stores each week according to the pattern:

$$\ldots\text{SSTTSTSSSTSTTT}\ldots$$

$$P = \begin{array}{c} S \\ T \end{array} \begin{pmatrix} 0.7 & 0.3 \\ 0.2 & 0.8 \end{pmatrix} \leftarrow \text{ irreducible}$$

One can find the answer for π by using *detailed balance.* In equilibrium, the number of customers swapping $T \to S$ is exactly balanced by customers $S \to T$.

$$\begin{array}{rl} \pi_T p_{TS} = & \pi_S p_{ST} \\ \text{Tesco} \to \text{Sainsbury} & \text{Sainsbury} \to \text{Tesco} \\ T(\text{loss}) & T(\text{gain}) \end{array}$$

Equivalently

$$\begin{aligned} S(\text{loss to Tesco}) &= S(\text{gain from Tesco}) \\ \pi_T 0.2 &= \pi_S 0.3 \\ \pi_T &= 1.5\pi_S \end{aligned}$$

The additional equation that we employ is the *normalisation* of the distribution:

$$\begin{aligned} \pi_S + \pi_T &= 1 \\ \Rightarrow \pi_S + 1.5\pi_S &= 1 \\ \pi_S &= 0.4 \\ \pi_T &= 0.6 \\ \Rightarrow \text{ On 1 week of sales Tesco } &60\% \text{ of market} \\ \text{Sainsbury } &40\% \text{ of market} \end{aligned}$$

By the *ergodic theorem* this means that a single shopper spends 60% of their time at Tesco (that is they shop at Tesco 6 weeks out of 10). Note that this idea of equilibrium (also called stationarity) does not mean the process is static. Rather it means that we have a dynamic equilibrium in which the fluctuations and changes even out over time. This is the concept of the law of large numbers applied in which the large sample limit is the long-time limit.

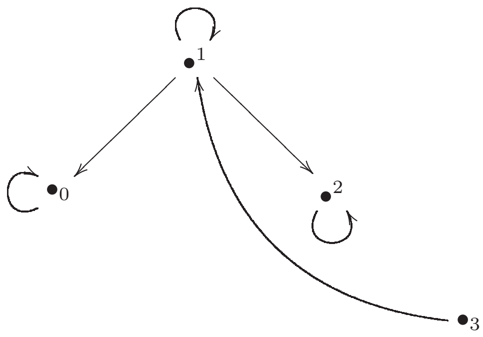
Again, by the ergodic theorem we can calculate the *recurrence time* - the expected time of return.

That is, if a single customer shops at Tesco this week; on average, when will they return to Tesco?

$$\mu_T = \frac{1}{\pi_T} = \frac{1}{0.6} = 1.67 \text{ weeks.}$$

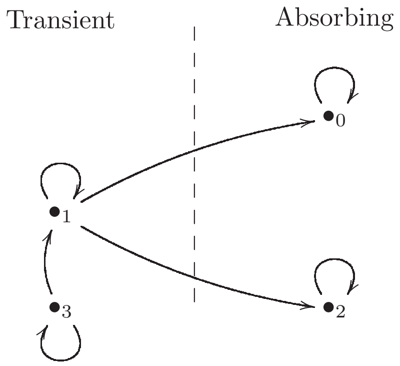
16.2 Transient and Absorbing States

Suppose that there is a Markov chain consisting of only transient and absorbing states (all recurrent states are absorbing). For example



In this case the states 0, 2 only have 1 outgoing edges (arrows) and these returned to the original state. {0,2} are clearly absorbing states (once they are reached, the system never leaves that state). {1,3} are *transient* states - that is, there is a *finite* probability that, once the state is left, it *never* returns to that state.

We can partition the states into 2 classes



In this section we address the following questions:

1. Starting from any *transient state*, j, what is the probability of finishing in any absorbing state, α?

   This is called the *hitting probability*, and to answer this question we will use the partition rule in the form:
$$P(A) = \sum_i P(A|B_i)P(B_i) \qquad , \tag{16.8}$$
   where A is the event starting from a given transient state j, one finishes (in the long run) in the absorbing state, α, and we condition on the first step, B.

   The question we pose is simply a generalisation of the gambler's ruin problem in which the aim was to calculate the probability of ruin. Starting from a given state, the probability that the series of games/steps ends with either ruin or fortune. That is, the transient states are defined by $x = k$, the amount of money the gambler begins with. The two absorbing states are $x = 0$ and $x = N$, that is the game always ends, eventually, with either ruin or fortune.

2. Starting from any transient state, j, what is the average time until the Markov process terminates?

This is called the *hitting time*, and to solve this problem we employ the and the conditional expectation theorem:

$$\mathbb{E}\left(Y\right) = \mathbb{E}\left(\mathbb{E}\left(Y|X\right)\right) \qquad . \tag{16.9}$$

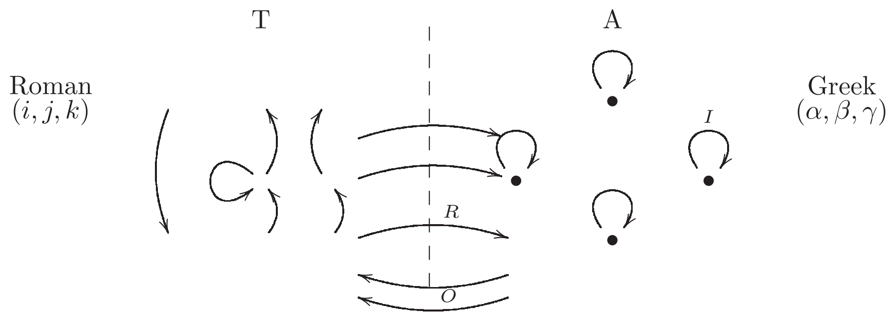
Again, with reference to the gambler's ruin problem, this corresponds to the expected duration of the random walk, that is the expected number of steps until the game terminates with either ruin or fortune.

We'll use Greek letters $(\alpha, \beta, \gamma, \dots)$ to label the absorbing states, and Latin letters $(i, j, k, \dots)$ for the transient states, and partition the transition matrix with the N_T transient states allocated to the first N_T rows, and the following N_A rows reserved for the absorbing states. Therefore the top-left block $(N_T \times N_T)$ of the transition matrix contain the elements that define the transitions between the transient states. Similarly, the bottom-right $(N_A \times N_A)$ square block of the transition matrix involve only the absorbing states.

Recalling the characteristics of absorbing states - in the transition matrix $p_{\alpha\alpha} = 1$ all other element are zero in the same row.

$$P = \begin{array}{c} \text{Transient} \\ \\ \text{Absorbing} \end{array} \left(\begin{array}{ccccccccc} & & & & \vdots & & & & \\ & & & & \vdots & & & & \\ & & & & \vdots & & & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \vdots & 1 & & & \\ 0 & 0 & 0 & 0 & \vdots & & 1 & & \\ 0 & 0 & 0 & 0 & \vdots & & & 1 & \end{array} \right) \Big\} N \text{ state}$$

$$P = \begin{array}{c} \text{Transient} \\ \\ \text{Absorbing} \end{array} \begin{pmatrix} \mathrm{Q} & \vdots & \mathrm{R} \\ \cdots & \cdots & \cdots \\ \mathrm{O} & \vdots & \mathrm{I} \end{pmatrix} \begin{array}{l} \} \; N_T \\ \\ \} \; N_A \end{array} \quad N_T + N_A = N$$



16.2.1 Hitting probability

Given that, starting from any transient state, $j \in T$, we finish up (eventually) in an absorbing state $\alpha \in A$, the question is, what is the probability of ending up (terminating the process) in a particular *absorbing state*. This is called the *hitting probability* for state α starting from state j:

$$H_{j\alpha} = P(X_\infty = \alpha | X_0 = j) \quad . \tag{16.10}$$

Note that this *hitting matrix* has N_T rows corresponding to $j \in T$, but N_A columns corresponding to $\alpha \in A$. So in general, it is rectangular.

Trivially, if one starts from one of the absorbing states, one is certain to remain there, that is:

$$\boxed{H_{\alpha\beta} = \delta_{\alpha\beta}} \quad , \tag{16.11}$$

where we use the Kronecker delta notation:

$$\delta_{\alpha\beta} = \begin{cases} 1 & , \quad \alpha = \beta \\ 0 & , \quad \alpha \neq \beta \end{cases} \quad , \tag{16.12}$$

We are not very interested in this part of the hitting matrix, as the answer is obvious.

To calculate the other block of the hitting matrix, we try the usual trick of conditioning on the first step. This gives us:

$$\begin{aligned} H_{j\alpha} &= P(X_\infty = \alpha | X_0 = j) && (16.13) \\ &= \sum_{k=1}^{N} P(X_\infty = \alpha | X_1 = k, X_0 = j) P(X_1 = k | X_0 = j) && (16.14) \\ &= \sum_{k=1}^{N} P(X_\infty = \alpha | X_1 = k) P(X_1 = k | X_0 = j) && (16.15) \\ & && (16.16) \end{aligned}$$

where we have used the Markovian property that the past can be ignored:

$$P(X_\infty = \alpha | X_1 = k, X_0 = j) = P(X_\infty = \alpha | X_1 = k) \quad .$$

Since the Markov chain is homogeneous, and adding/subtracting 1 from ∞ makes no difference to ∞, we have:

$$P(X_\infty = \alpha | X_1 = k) = P(X_\infty = \alpha | X_0 = k) = h_{k\alpha} \quad . \tag{16.17}$$

This leads to:

$$\boxed{H_{j\alpha} = \sum_{k=1}^{N} p_{jk} H_{k\alpha}} \quad . \tag{16.18}$$

This represents are set of linear equations for the unknown quantities we seek, the *hitting probabilities*: $h_{j\alpha}$. We can divide the sum in two corresponding to the partitioning of the transition matrix:

$$\mathsf{P} = \begin{pmatrix} \mathsf{Q} & \mathsf{R} \\ 0 & \mathsf{I} \end{pmatrix} \quad , \tag{16.19}$$

so that equation (16.18) can be written as:

$$H_{j\alpha} = \sum_{k\in T} Q_{jk} H_{k\alpha} + \sum_{\beta\in A} R_{j\beta} H_{\beta\alpha} \quad . \tag{16.20}$$

Given that (16.11) this further simplifies to:

$$\boxed{H_{j\alpha} = \sum_{k\in T} Q_{jk} H_{k\alpha} + R_{j\alpha}} \quad . \tag{16.21}$$

This equation corresponds to the generalisation of the simple random walk equation that we discussed earlier:

$$p_k = pp_{k+1} + qp_{k-1} \quad . \tag{16.22}$$

However, the connection between the two it is not immediately obvious!

Since these are linear equations, we can write them using matrix notation (shorthand):

$$\mathsf{H} = \mathsf{QH} + \mathsf{R} \quad . \tag{16.23}$$

Rearranging this gives us:

$$(\mathsf{I} - \mathsf{Q})\mathsf{H} = \mathsf{R} \quad , \tag{16.24}$$

with the solution (if the inverse exists):

$$\boxed{\mathsf{H} = (\mathsf{I} - \mathsf{Q})^{-1}\mathsf{R}} \tag{16.25}$$

The matrix:

$$\mathsf{N} \equiv (\mathsf{I} - \mathsf{Q})^{-1} \quad , \tag{16.26}$$

is called the *fundamental matrix*. The meaning of this expression becomes clear if we consider the series expansion, within its radius of convergence, of the fundamental matrix:

$$(\mathsf{I} - \mathsf{Q})^{-1} = \mathsf{I} + \mathsf{Q} + \mathsf{Q}^2 + \mathsf{Q}^3 + \cdots \quad .$$

To confirm that this expansion is valid, simply multiply both left and right-hand sides by the matrix:$\mathsf{I} - \mathsf{Q}$. Using this expansion leads to the series expression:

$$\mathsf{H} = \mathsf{R} + \mathsf{QR} + \mathsf{Q}^2\mathsf{R} + \mathsf{Q}^3\mathsf{R} + \cdots \quad . \tag{16.27}$$

The first term on the right-hand side, R, represents a one-step (direct) transition from the transient to the absorbing state. The second term, QR, includes all processes that have the first step in the transient set before the second step into the absorbing set. The third term, $\mathsf{Q}^2\mathsf{R}$, has *two steps* in the transient state space before the third step into the absorbing sets. In principle there is an infinity of such jumps before absorption. The higher order terms represents all the other higher order processes. That is, we are taking into account all possible pathways from the transient state to the absorbing states, and adding all the associated probabilities.

So the matrix inversion, the calculation of the fundamental matrix (16.26), allows one to take all of these terms into account.

16.2.2 Hitting Time

Given that the transient states eventually terminate in the absorbing states, a natural question to ask is how long does such a process take. The number of steps for such a process is, of course, random since the transitions are random.

However, we can estimate the *expected value* of this time: called the hitting time. So for each transient state $j \in T$, we have the number of steps to absorption:

$$Y_j = \min\{n : X_n \in A, X_0 = j\} \quad . \tag{16.28}$$

Clearly if $j \in A$, that is, if we start from an absorbing state, then the number of steps (time to absorption) is zero:

$$Y_j = 0 \qquad j \in A \quad . \tag{16.29}$$

Let $\mathbb{E}(Y_j) = y_j$ denote the expected value of the *hitting time* starting from the transient state j.

We use the established idea of the *conditional expectation theorem*, conditioning on the first step. So we start at $X_0 = j$, which is known and then jump randomly to state $X_1 = k$ on the first transition. So to calculate $\mathbb{E}(Y_j)$ we try the following:

$$\boxed{\mathbb{E}(Y_j) = \mathbb{E}(\mathbb{E}(Y_j|X_1))} \quad . \tag{16.30}$$

Now:

$$\mathbb{E}(\mathbb{E}(Y_j|X_1)) = \sum_{k=1}^{N} \mathbb{E}(Y_j|X_1 = k, X_0 = j) P(X_1 = k|X_0 = j) \quad , \tag{16.31}$$

where the state k could be either $k \in A, T$. Furthermore, by definition:

$$P(X_1 = k|X_0 = j) = p_{jk} \quad . \tag{16.32}$$

Then we have that, if the first step takes us directly into an absorbing state:

$$\mathbb{E}(Y_j|X_1 = k, X_0 = j) = 1 \quad , \quad k \in A \tag{16.33}$$

while for $k \in T$

$$\mathbb{E}(Y_j|X_1 = k, X_0 = j) = 1 + \mathbb{E}(Y_k) = 1 + y_k \quad . \tag{16.34}$$

The last equation deserves some explanation. If our first step is towards another transient state k, then we have used up 1 step (one unit of time) and now the expected time is the hitting time starting from the new state, k. Putting all these ideas together we find that (16.31) now has the simple form:

$$y_j = \sum_{k \in T} p_{jk}(1 + y_k) + \sum_{k \in A} p_{jk} \quad . \tag{16.35}$$

Since:

$$\sum_{k \in A, T} p_{jk} = 1 \quad ,$$

for any j. This simplifies to the result:

$$y_j = 1 + \sum_{k \in T} p_{jk} y_k = 1 + \sum_{k \in T} Q_{jk} y_k \quad . \tag{16.36}$$

Thus the only part of the transition matrix involved is the upper left corner, the part involving the transient states, Q.

Note that this relation is simply the generalisation of the simple random walk difference equation for the duration of the walk:

$$\underbrace{d_k}_{\substack{\text{expected time to absorption} \\ \text{(duration of walk/hitting time)}}} = 1 + pd_{k+1} + qd_{k-1} \tag{16.37}$$

The relation (16.36) is a set of N_T linear equations, since $j = 1, 2, \ldots, N_T$. It is more convenient, mathematically, to express this equation in matrix form. So let us define a column vector with N_T rows:

$$\mathsf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N_T} \end{pmatrix} \quad . \tag{16.38}$$

Recalling that Q_{jk} is an $N_T \times N_T$ square matrix of the transient states $j, k \in T$, then we can write (16.36) in the form:

$$\mathsf{y} = \mathsf{e} + \mathsf{Q}\mathsf{y} \quad , \tag{16.39}$$

where we use the shorthand, for the column vector e, with N_T rows:

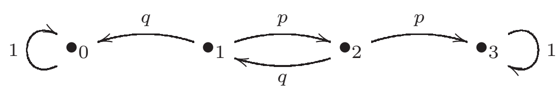
$$\mathsf{e} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \quad . \tag{16.40}$$

After a bit of rearrangement of (16.39), this simplifies to the final result:

$$\boxed{\mathsf{y} = (\mathsf{I} - \mathsf{Q})^{-1}\mathsf{e}} \quad . \tag{16.41}$$

Thus each element of the column y will give individual hitting times for each of the transient states.

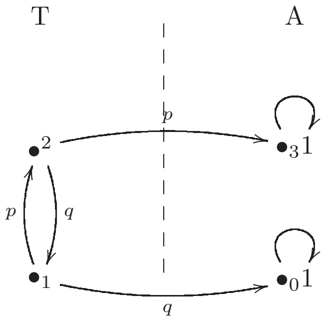
Example: Consider the chain



(Gambler's ruin $N = 3$ in disguise).

1. Find the transient states

2. Obtain an expression for the hitting probabilities for each transient state. Find the probability that, given one starts in state 1, that the random process will terminate in state 3.



$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ q & 0 & p & 0 \\ 0 & q & 0 & p \\ 0 & 0 & 0 & 1 \end{pmatrix} \{1,2\}\mathrm{T} : \{0,4\}\mathrm{A}$$

$$\begin{array}{cc} & \begin{array}{ccccc} \mathrm{T} & & & \mathrm{A} & \end{array} \\ \begin{array}{cc} & 1 \\ \mathrm{T} & 2 \\ \mathrm{A} & 0 \\ & 3 \end{array} & \begin{pmatrix} & & \vdots & & \\ & & \vdots & & \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \vdots & 1 & 0 \\ 0 & 0 & \vdots & 0 & 1 \end{pmatrix} \end{array} \rightarrow \begin{array}{cc} & \begin{array}{ccccc} \mathrm{T} & & & \mathrm{A} & \end{array} \\ \begin{array}{cc} & 1 \\ \mathrm{T} & 2 \\ \mathrm{A} & 0 \\ & 3 \end{array} & \begin{pmatrix} 0 & p & \vdots & q & 0 \\ q & 0 & \vdots & 0 & p \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \vdots & 1 & 0 \\ 0 & 0 & \vdots & 0 & 1 \end{pmatrix} \end{array}$$

Then

$$\mathsf{Q} = \begin{pmatrix} 0 & p \\ q & 0 \end{pmatrix} \quad , \quad \mathsf{R} = \begin{pmatrix} q & 0 \\ 0 & p \end{pmatrix} \quad .$$

Recall that the *hitting matrix* is given by the expression:

$$\begin{aligned} \mathsf{H} &= (\mathsf{I} - \mathsf{Q})^{-1}\mathsf{R} \\ &= \left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & p \\ q & 0 \end{pmatrix} \right]^{-1} \begin{pmatrix} q & 0 \\ 0 & p \end{pmatrix} \\ &= \begin{pmatrix} 1 & -p \\ -q & 1 \end{pmatrix}^{-1} \begin{pmatrix} q & 0 \\ 0 & p \end{pmatrix} \end{aligned}$$

$$\begin{aligned} \mathsf{H} &= \frac{1}{1-pq} \begin{pmatrix} 1 & p \\ q & 1 \end{pmatrix} \begin{pmatrix} q & 0 \\ 0 & p \end{pmatrix} \\ &= \frac{1}{1-pq} \begin{pmatrix} q & p^2 \\ q^2 & p \end{pmatrix} \end{aligned}$$

Then, in particular, we have that (first row, second column) and (first row, first column):

$$H_{13} = \frac{p^2}{1-pq} \quad , \quad H_{10} = \frac{q}{1-pq} \quad . \tag{16.42}$$

We also have, taking the *second row* of the hitting matrix:

$$H_{23} = \frac{p}{1-pq} \quad , \quad H_{20} = \frac{q^2}{1-pq} \quad . \tag{16.43}$$

So this tells us the probabilities of the transient states hitting the two absorbing states.

We can also verify that $H_{10} + H_{13} = 1$. This equation means that the probability that (starting at 1) one ends up with either 0 or 3, eventually. This is always the fate of a Markov chain that starts in a transient state, it will eventually terminate in one the absorbing states (or recurrent states).

In this can we note that:

$$H_{10} + H_{13} = \frac{q}{1-pq} + \frac{p^2}{1-pq} \tag{16.44}$$

Then, recalling that $p + q = 1$, for the gambler's ruin problem:

$$\frac{q+p^2}{1-pq} = \frac{q+p(1-q)}{1-pq} = \frac{1-pq}{1-pq} = 1 \quad . \tag{16.45}$$

In a similar manner we can show that: $H_{20} + H_{23} = 1$.

Finally, one can calculate the *hitting times* for this Markov chain using the formula (**??**).

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \frac{1}{1-pq} \begin{pmatrix} 1 & p \\ q & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad . \tag{16.46}$$

Thus, the expected time to absorption, that is the duration of the process, is given by

$$y_1 = \frac{1+p}{1-pq} \quad , \quad y_2 = \frac{1+q}{1-pq} \quad . \tag{16.47}$$

when starting from 1 or 2, respectively. Just as a quick check, suppose the process was not random at all, and that $p = 0$ and $q = 1$. Then the Gambler would lose every game with certainty. According to our formulae (16.47), we would predict: $y_1 = 1$ and $y_2 = 2$, which is exactly what one would expect.