THE FUNDAMENTAL MATRIX OF THE GENERAL RANDOM WALK WITH ABSORBING BOUNDARIES

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Abstract. The general random walk on the nonnegative integers with absorbing boundaries at 0 and n has the transition probabilities $p_{0j} = \delta_{0j}$, $p_{nj} = \delta_{nj}$, $p_{i,i-1} = p_i$, $p_{i,i+1} = q_i$, and $p_{ii} = r_i$, where $p_i + r_i + q_i = 1$. The fundamental matrix B of this Markov chain is the inverse of matrix $(I - Q)$ where Q results from P by deleting the rows and columns 0 and n. Entry b_{ij} represents the expected number of occurrences of the transient state j prior to absorption if the random walk starts at state i. The absorption time as well as the absorption probabilities are easily derived once the fundamental matrix is known. Here, it is shown that the fundamental matrix can be determined in elementary manner via the adjugate of matrix $(I - Q)$.

Key words. General random walk, fundamental matrix, absorption times, absorption probability

AMS subject classifications. 60J15, 60J20

1. Introduction. Random walk models have surfaced in various disciplines. They served as initial simple models in biology (especially in genetics) and physics, but they are also useful tools in analyzing sequential test procedures in statistics or randomized algorithms in computer science—to name only few fields of application.

Needless to say, many results have been published for specific instantiations of the transition probabilities; the general case, however, seems to be explored with less intensity. For example, El-Shehawey [1] has determined the joint probability generating function of the number of occurrencies of the transient states. Its marginals may be used to derive the fundamental matrix but the expression offered in [1] contains unresolved recurrence relations that make potential further calculations difficult. Therefore, this work aims at a 'closed form' expression for each entry of the fundamental matrix. It will be shown that such a result can be achieved via elementary matrix theory.

2. General Random Walk with Absorbing Boundaries. At first, some notation being adopted from Minc [2] is introduced. Next, the Markov chain model of the random walk is presented along with some basic results from Markov chain theory taken from Iosifescu [3]. Finally, the fundamental matrix of the Markov chain as well as expressions for the absorption time and absorption probabilities are determined.

2.1. Notation. Let A be an $m \times n$ matrix. Then $A(\alpha_1, \ldots, \alpha_h | \beta_1, \ldots, \beta_k)$ denotes the $(m-h) \times (n-k)$ submatrix of A obtained from A by deleting rows $\alpha_1, \ldots, \alpha_h$ and columns $\beta_1, \ldots, \beta_k$ whereas $A[\alpha_1, \ldots, \alpha_h | \beta_1, \ldots, \beta_k]$ denotes the $h \times k$ submatrix of A whose (i, j) entry is a_{α_i, β_j}. If $\alpha_i = \beta_i$ for $i = 1, \ldots, k$ then the shorthand notation $A(\alpha_1, \ldots, \alpha_k)$ resp. $A[\alpha_1, \ldots, \alpha_k]$ will be used. As usual, A^{-1} is the inverse and $\det A$ is the determinant of a regular square matrix A. Matrix I is the unit matrix and every entry of column vector e is 1.

2.2. Markov Chain Model. The general random walk with absorbing boundaries is a time-homogeneous Markov chain $(X_k : k \geq 0)$ with state space $\{0, 1, \ldots, n\}$

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and transition matrix

$$P = \begin{pmatrix} 1 & 0 & 0 & \cdots & & & 0 \\ p_1 & r_1 & q_1 & 0 & \cdots & & 0 \\ 0 & p_2 & r_2 & q_2 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & p_{n-2} & r_{n-2} & q_{n-2} & 0 \\ 0 & \cdots & & 0 & p_{n-1} & r_{n-1} & q_{n-1} \\ 0 & \cdots & & & 0 & 0 & 1 \end{pmatrix}$$

such that $\mathsf{P}\{ X_{k+1} = j \mid X_k = i \} = p_{ij}$ for $i, j = 0, 1, \ldots, n$. Let $Q = P(0, n)$, i.e., Q results from P by deleting the rows and columns 0 and n, and set $A = I - Q$. Then $B = A^{-1}$ is the fundamental matrix associated with the transition matrix P. Let $T = \min\{ k \geq 0 : X_k \in \{0, n\}\}$. Then $\mathsf{E}[\, T \mid X_0 = i \,] = a_i$ denotes the absorption time for a random walk starting at state i where a_i is the ith entry of vector $a = Be$. Thus, a_i is just the sum of all entries of row i of the fundamental matrix. In case of the random walk, the absorption probabilities are $\mathsf{P}\{ X_T = 0 \mid X_0 = i \} = b_{i1} \cdot p_{10}$ and $\mathsf{P}\{ X_T = n \mid X_0 = i \} = b_{i,n-1} \cdot p_{n-1,n}$ for $i = 1, \ldots, n-1$.

2.3. Determination of the Fundamental Matrix. There are many methods to obtain the inverse of some regular square matrix. Here, the inverse of matrix $(I - Q)$ is determined via its adjugate. This approach is especially useful if only few elements of the inverse are of interest.

Let $A : d \times d$ be a regular square matrix. The adjugate $\operatorname{adj}(A)$ of matrix A is the matrix whose (i, j) entry is $(-1)^{j+i} \det A(j|i)$. Since $B = A^{-1} = \operatorname{adj}(A)/\det(A)$ one obtains

$$b_{ij} = (-1)^{i+j} \, \frac{\det A(j|i)}{\det A}$$

for $i, j = 1, \ldots, d$. To proceed one needs an elementary expression for the determinant of matrix A.

LEMMA 2.1. *Let P be the transition matrix of the general random walk with absorbing boundaries at state 0 and state n. Let $Q = P(0, n)$ and set $A_d = I - Q$ with $d = n - 1$. The determinant of A_d is given by*

$$\det A_d = \sum_{k=0}^{d} \left(\prod_{i=1}^{d-k} p_i \right) \left(\prod_{j=d-k+1}^{d} q_j \right)$$

for all $d \geq 1$.

Proof. (by induction)
Let $d = 1$. Then matrix A_d reduces to $A_1 = (p_1 + q_1)$ with $\det A_d = p_1 + q_1$. Since

$$\sum_{k=0}^{1} \left(\prod_{i=1}^{1-k} p_i \right) \left(\prod_{j=2-k}^{1} q_j \right) = p_1 + q_1$$

the hypothesis is true for $d = 1$. Now let $d = 2$. The determinant of matrix A_2 is

$$\det A_2 \;=\; \det \begin{pmatrix} p_1 + q_1 & -q_1 \\ -p_2 & p_2 + q_2 \end{pmatrix} \;=\; p_1\, p_2 + p_1\, q_2 + q_1\, q_2 \,.$$

Since

$$\sum_{k=0}^{2} \left(\prod_{i=1}^{2-k} p_i \right) \left(\prod_{j=3-k}^{2} q_j \right) = p_1\, p_2 + p_1\, q_2 + q_1\, q_2$$

the hypothesis is true for $d = 2$ as well. Suppose that the hypothesis is true for $d-1$ and d for $d \geq 2$. The determinant of matrix A_{d+1} can be expressed in terms of $\det A_d$ and $\det A_{d-1}$ via

$$\begin{aligned}
\det A_{d+1} &= \det \begin{pmatrix} \boxed{\quad A_d \quad} & \begin{matrix} \\ -q_d \end{matrix} \\ \begin{matrix} \qquad & -p_{d+1} \end{matrix} & p_{d+1} + q_{d+1} \end{pmatrix} \\
&= \det \begin{pmatrix} \boxed{A_{d-1}} & \begin{matrix} \\ -q_{d-1} \end{matrix} & \\ \begin{matrix} \qquad & -p_d \end{matrix} & p_d + q_d & -q_d \\ & -p_{d+1} & p_{d+1} + q_{d+1} \end{pmatrix} \\
&= (p_{d+1} + q_{d+1}) \det A_d + p_{d+1} \det \begin{pmatrix} \boxed{A_{d-1}} & \begin{matrix} 0 \\ \vdots \\ 0 \end{matrix} \\ \begin{matrix} \qquad & -p_d \end{matrix} & -q_d \end{pmatrix} \\
&= (p_{d+1} + q_{d+1}) \det A_d - p_{d+1}\, q_d \det A_{d-1} \\
&= q_{d+1} \det A_d + p_{d+1} \left(\det A_d - q_d \det A_{d-1} \right). \qquad (2.1)
\end{aligned}$$

By hypothesis, one obtains

$$\begin{aligned}
q_{d+1} \det A_d &= q_{d+1} \sum_{k=0}^{d} \left(\prod_{i=1}^{d-k} p_i \right) \left(\prod_{j=d-k+1}^{d} q_j \right) \\
&= \sum_{k=0}^{d} \left(\prod_{i=1}^{d-k} p_i \right) \left(\prod_{j=d-k+1}^{d+1} q_j \right) \qquad (2.2) \\
&= \sum_{k=1}^{d+1} \left(\prod_{i=1}^{d+1-k} p_i \right) \left(\prod_{j=(d+1)-k+1}^{d+1} q_j \right) \qquad (2.3)
\end{aligned}$$

where eqn. (2.3) results from an index shift in eqn. (2.2). The same arguments yield

$$q_d \det A_{d-1} = \sum_{k=1}^{d} \left(\prod_{i=1}^{d-k} p_i \right) \left(\prod_{j=d-k+1}^{d} q_j \right)$$

and hence

$$p_{d+1} \left(\det A_d - q_d \det A_{d-1} \right) = \prod_{i=1}^{d+1} p_i\,. \qquad (2.4)$$

Insertion of eqns. (2.3) and (2.4) into eqn. (2.1) leads to

$$\begin{aligned}\det A_{d+1} &= \sum_{k=1}^{d+1}\left(\prod_{i=1}^{d+1-k} p_i\right)\left(\prod_{j=(d+1)-k+1}^{d+1} q_j\right) + \prod_{i=1}^{d+1} p_i \\ &= \sum_{k=0}^{d+1}\left(\prod_{i=1}^{(d+1)-k} p_i\right)\left(\prod_{j=(d+1)-k+1}^{d+1} q_j\right)\end{aligned}$$

which is the desired result. □

Next, one needs an elementary expression for the determinant of $A(j|i)$. The first step in this direction is similar to the approach in Minc [2, pp. 147–149] who considered the more general case of establishing a general expression for a submatrix of a tridiagonal matrix. Here, the situation is less complicated. Since submatrix $A(j|i)$ results from the tridiagonal matrix A after the deletion of row j and column i, the submatrix is in lower triangular block form if $i < j$, in diagonal block form if $i = j$, and in upper triangular block form if $i > j$. Each of these "blocks" is a square submatrix of A. Notice that the determinant of such block matrices is the product of the determinants of the diagonal blocks. As a consequence, one obtains

$$\det A(j|i) = \det(A[1,\dots,i-1]) \cdot \det(A[i,\dots,j-1 \,|\, i+1,\dots,j]) \cdot \det(A[j+1,\dots,d])$$

if $1 \le i < j \le d = n-1$,

$$\det A(j|i) = \det(A[1,\dots,i-1]) \cdot \det(A[j+1,\dots,d])$$

if $1 \le i = j \le d$, and

$$\det A(j|i) = \det(A[1,\dots,j-1]) \cdot \det(A[j+1,\dots,i \,|\, j,\dots,i-1]) \cdot \det(A[i+1,\dots,d])$$

if $1 \le j < i \le d$. As a convention, if $u > v$ then $\det(A[u,\dots,v]) = 1$.

The final step towards an elementary expression of $\det A(j|i)$ requires the determination of the determinants of the diagonal block matrices. An elementary expression for the matrices of the type $A[1,\dots,\ell]$ can be taken directly from Lemma 2.1. Since the structure of the matrices of the type $A[\ell+1,\dots,d]$ is identical to the structure of the matrices of the type $A[1,\dots,d-\ell]$, Lemma 2.1 also leads to an elementary expression for the determinants of these matrices—one must only take into account that the indices have the offset ℓ. Consequently, one obtains

$$\det A[\ell+1,\dots,d] = \sum_{k=0}^{d-\ell}\left(\prod_{u=\ell+1}^{d-k} p_u\right)\left(\prod_{v=d-k+1}^{d} q_v\right).$$

If $1 \le i < j \le d$ then matrix $A[i,\dots,j-1 \,|\, i+1,\dots,j]$ reduces to a lower triangular matrix. Similarly, if $1 \le j < i \le d$ then matrix $A[j+1,\dots,i \,|\, j,\dots,i-1]$ is upper triangular. It follows that

$$\det A[i,\dots,j-1 \,|\, i+1,\dots,j] = (-1)^{j-i}\prod_{k=i}^{j-1} q_k \qquad (1 \le i < j \le d)$$

and

$$\det A[j+1,\dots,i \,|\, j,\dots,i-1] = (-1)^{i-j}\prod_{k=j+1}^{i} p_k \qquad (1 \le j < i \le d).$$

Consequently, it has been proven:

THEOREM 2.2. *Let $B : (n-1)\times(n-1)$ be the fundamental matrix of the general random walk with absorbing boundaries at states 0 and n. The entries b_{ij} of matrix B are*

$$b_{ij} = \frac{\left[\sum_{k=0}^{i-1}\left(\prod_{u=1}^{i-k-1} p_u\right)\left(\prod_{v=i-k}^{i-1} q_v\right)\right] \times \left[\prod_{k=i}^{j-1} q_k\right] \times \left[\sum_{k=0}^{n-j-1}\left(\prod_{u=j+1}^{n-k-1} p_u\right)\left(\prod_{v=n-k}^{n-1} q_v\right)\right]}{\sum_{k=0}^{n-1}\left(\prod_{u=1}^{n-k-1} p_u\right)\left(\prod_{v=n-k}^{n-1} q_v\right)}$$

for $1 \le i \le j \le n-1$ and

$$b_{ij} = \frac{\left[\sum_{k=0}^{j-1}\left(\prod_{u=1}^{j-k-1} p_u\right)\left(\prod_{v=j-k}^{j-1} q_v\right)\right] \times \left[\prod_{k=j+1}^{i} p_k\right] \times \left[\sum_{k=0}^{n-i-1}\left(\prod_{u=i+1}^{n-k-1} p_u\right)\left(\prod_{v=n-k}^{n-1} q_v\right)\right]}{\sum_{k=0}^{n-1}\left(\prod_{u=1}^{n-k-1} p_u\right)\left(\prod_{v=n-k}^{n-1} q_v\right)}$$

for $n-1 \ge i > j \ge 1$. $\square$

Thanks to Theorem 2.2 one obtains the absorption time and probability via

$$\mathsf{E}[T \mid X_0 = i] = \sum_{j=1}^{n-1} b_{ij} \quad \text{resp.} \quad \mathsf{P}\{X_T = n \mid X_0 = i\} = b_{i,n-1}\cdot q_{n-1}$$

where $i = 1,\ldots,n-1$. As expected, these expressions reduce to well-known formulas if $p_i = p$ and $q_i = q$ for $i = 1,\ldots,n-1$. If $p = q$ then the limit operation $(q/p) \to 1$ is necessary.

3. Conclusions. Closed form expressions for the entries of the fundamental matrix of the general random walk with absorbing boundaries have been derived by means of elementary matrix theory. This leads also to closed form expressions for the absorption time and the absorption probabilities. The approach taken here is especially useful if, for example, the absorption time or the absorption probabilities for a specific initial state are of interest because only few entries of the fundamental matrix must be determined in this case.

REFERENCES

[1] M. A. El-Shehawey. On the frequency count for a random walk with absorbing boundaries: a carcinogenesis example. I. *J. Phys. A*, 27:7035–7046, 1994.
[2] H. Minc. *Nonnegative Matrices.* Wiley, New York, 1988.
[3] M. Iosifescu. *Finite Markov Processes and Their Applications.* Wiley, Chichester, 1980.