International Journal of Difference Equations (IJDE).
ISSN 0973-6069 Volume 2 Number 2 (2007), pp. 177–186

http://www.ripublication.com/ijde.htm

A Combinatorial Approach to Discrete Diffusion on a Segment

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Abstract

We find the solution of the partial difference equation

$$u(x, t + 1) = l\ u(x + 1, t) + r\ u(x - 1, t)$$

for $x \in [1, m]$ subject to the absorbing boundary conditions at $x = 0$ and $x = m+1$. Green's function will be determined using random walk techniques applying the reflective and inclusion-exclusion principles.

AMS subject classification: 39A12, 37H10.
Keywords: Partial difference equations, Green's function, random walks, reflective principle, inclusion-exclusion principle.

1. Preliminaries

Mathematical models in the biological and ecological sciences frequently use random walks to describe movement as well as population dynamics, see [2,5,7] for descriptions, examples and applications. Closed form solutions in the absence of boundary conditions are very easy to obtain on a discrete lattice using elementary counting techniques and when there is at most a single boundary condition for each direction in the lattice one can apply the reflective principle to obtain closed form solutions, see Avery and Berman [1] for further details. The approach we have taken in this paper is very algorithmic and yields a closed form solution for movement in the presence of two boundary conditions in one direction (for example, bounded above and below on a segment).

Received February 21, 2007; Accepted June 9, 2007

The problem as stated is similar to the gambler ruin problem. If one is only interested in the absorbed quantities on the boundary, then the problem is the standard gambler ruin problem which can be rephrased as a first order linear difference equation with constant coefficients which is easy to solve, see Kelley and Peterson [6] for a thorough treatment. The problem as stated can be solved by standard linear algebra methods by letting $U(t)$ be the $(m+2) \times 1$ column vector $[u(x,t)]$, then rewriting the problem as

$$U(t+1) = MU(t)$$

for the appropriate tridiagonal matrix M which in essence corresponds to the transitional technique, see Cheng [4] for a thorough treatment. The advantage of the combinatorial techniques applied in this paper is that regardless of the value of m, the closed form solution of the boundary value problem is attained and we can use this solution as a directional component of a solution in other random walk problems. That is, the techniques in this paper are transferable to random walks in the plane or higher dimensions when one of the components of the environment is bounded above and below. For example, one can use the results of this paper to determine Green's function for a random walk on a strip or in a rectangle of the plane with absorbing boundary conditions. Furthermore, information concerning the solution is encoded in Green's function which corresponds to the number of walks on the segment with the appropriate initial and terminal conditions that avoid the boundary. The combinatorial solution has a random walk interpretation, an interpretation currently missing from the literature.

2. Introduction to Discrete Diffusion on a Segment

In this paper we will find the solution for discrete diffusion on a segment

$$u(x, t+1) = lu(x+1, t) + ru(x-1, t)$$

for $x \in [1, m]$ with absorbing boundary conditions. One can interpret u as representing the objects in a random walk on a line segment that are still moving, thus the absorbing boundary condition for u corresponds to

$$u(0, t) = 0 = u(m+1, t)$$

for all t and if we let v represent the objects that have been absorbed (not moving) in the random walk, then

$$v(0, t) = l \sum_{\tau=1}^{t-1} u(1, \tau)$$

and

$$v(m+1, t) = r \sum_{\tau=1}^{t-1} u(m, \tau).$$

3. Combinatorial Approach to find Green's Function

Define a one dimensional random walk as a movement on a discrete line (steps of size 1) with the property that regardless of the time the walker moves Right or the walker moves Left. Let $W(k, n, t)$ be the number of walks with initial location k that are at n at time t.

Lemma 3.1. If $t - |n - k|$ is nonnegative and even, then

$$W(k, n, t) = \binom{t}{\frac{t-|n-k|}{2}}.$$

Otherwise $W(k, n, t) = 0$.

Proof. If $n \geq k$, then any walk from k to n must have $n - k$ more Rights than Lefts, thus $t - (n - k)$ must be nonnegative (to have enough steps to go from k to n) and even (since for each additional Right in the walk there must be an additional Left in the walk). Thus any walk from k to n must have

$$\frac{t-(n-k)}{2} \text{ Lefts, and } \frac{t+(n-k)}{2} \text{ Rights}$$

and therefore the number of distinct walks from k to n in t steps is given by

$$W(k, n, t) = \binom{t}{\frac{t-(n-k)}{2}}$$

(choosing which of the t steps are Lefts and those that remain are Rights). The argument is identical if $k \geq n$ and $t - (k - n)$ is nonnegative and even in which case there are

$$\frac{t+(k-n)}{2} \text{ Lefts, and } \frac{t-(k-n)}{2} \text{ Rights}$$

and hence

$$W(k, n, t) = \binom{t}{\frac{t-(k-n)}{2}}$$

walks from k to n in t steps. Therefore, regardless of the relative position of the initial and terminal locations, we have

$$W(k, n, t) = \binom{t}{\frac{t-|n-k|}{2}}.$$

■

The key to determining Green's function for our problem is to determine how many walks avoid the boundary. Applying the inclusion-exclusion principle in conjunction with the reflective principle, we will determine the number of walks that reach the boundary of the segment. The following lemma is often referred to as André's reflection principle and can be found in Rosen's combinatorics handbook [8] as well as most other combinatorics texts.

Lemma 3.2. The number of walks that start at a positive integer k and finish at a positive integer m by increasing or decreasing by one unit at each step that are zero at some step in the course of taking an integer $t = u + d$ number of steps, where u is the number of ups and d is the number of downs, is the same as the number of walks from $-k$ to m in t steps with $u + k$ ups and $d - k$ downs.

The one-to-one correspondence between the two types of walks is established by reflecting the steps of the walks that lead to the first encounter with the boundary 0 about 0 (changing ups to downs and downs to ups for all of the steps that led to the first encounter with 0). Let $Z(t)$ be the number of walks from $m + 1$ to $m + 1$ in $t \geq 1$ steps that avoid the boundary 0.

Theorem 3.3. If $t \geq 1$ is even, then

$$Z(t) = \binom{t}{\frac{t}{2}} - \binom{t}{\frac{t}{2} + (m+1)}.$$

Otherwise $Z(t) = 0$.

Proof. Any walk with the same initial location as terminal location has the same number of Lefts as Rights in the walk. Thus if $Z(t)$ is nonzero, the number of steps taken must be even (twice the number of Lefts taken). If t is even, then any arrangement of $\frac{t}{2}$ Lefts and $\frac{t}{2}$ Rights corresponds to a distinct walk from $m + 1$ to $m + 1$, hence there are

$$\binom{t}{\frac{t}{2}}$$

distinct walks from $m + 1$ to $m + 1$. By the reflective principle, the number of walks from $m + 1$ to $m + 1$ in t steps that reach the boundary 0 at some step is the same as the number of walks from $-m - 1$ to $m + 1$ in t steps with $\frac{t}{2} - (m + 1)$ Lefts and $\frac{t}{2} + (m + 1)$ Rights, and there are

$$\binom{t}{\frac{t}{2} + (m+1)}$$

walks of this type. Therefore, if $t \geq 2$ is even, then the number of walks from $m + 1$ to $m + 1$ in t steps that avoid the boundary 0 is given by

$$Z(t) = \binom{t}{\frac{t}{2}} - \binom{t}{\frac{t}{2} + (m+1)}.$$

This concludes the proof. ■

For $k \in [1, m]$, let $S_k(t)$ be the number of walks from k to $m+1$ in $t \geq 1$ steps that avoid the boundary 0.

Theorem 3.4. If $t \geq 1$ and $t - (m+1-k)$ is nonnegative and even, then

$$S_k(t) = \binom{t}{\frac{t-(m+1-k)}{2}} - \binom{t}{\frac{t-(m+1+k)}{2}}.$$

Otherwise $S_k(t) = 0$.

Proof. Any walk with initial location k and terminal location $m+1$ in t steps must have $m+1-k$ more Rights than Lefts. Thus $t-(m+1-k)$ must be nonnegative and even. Moreover there are

$$\frac{t-(m+1-k)}{2} \quad \text{Lefts, and} \quad \frac{t+(m+1-k)}{2} \quad \text{Rights}$$

in any walk from k to $m+1$ in t steps. By the reflection principle, the number of walks from k to $m+1$ in t steps that reach the boundary 0 at a step before t is the same as the number of walks from $-k$ to $m+1$ in t steps with

$$\frac{t-(m+1+k)}{2} \quad \text{Lefts, and} \quad \frac{t+(m+1+k)}{2} \quad \text{Rights.}$$

Hence, there are

$$\binom{t}{\frac{t-(m+1-k)}{2}} - \binom{t}{\frac{t-(m+1+k)}{2}}$$

distinct walks from k to $m+1$ in t steps that avoid the boundary 0. ■

For $k \in [1, m]$ and $t \geq s \geq 1$, let $B_s(k, t)$ be the set of all walks from k to $m+1$ in t steps that avoid the boundary 0 and at time s are at the boundary $m+1$. Let $A_j(k, t)$ be the sum associated to j of the intersection properties, that is:

$$A_j(k, t) = \sum |B_{s_1}(k, t) \cap B_{s_2}(k, t) \cap \cdots \cap B_{s_j}(k, t)|,$$

where the sum is over all possible intersection times s_i with the property that

$$t > s_j > s_{j-1} > \cdots > s_1 \geq 1.$$

Theorem 3.5. For $k \in [1, m]$ and j a positive integer, if $t - (m+1-k)$ is even and $t - (m+1-k) \geq 2j$, then

$$A_j(k, t) = \sum_{z_1=0}^{u_1} \sum_{z_2=0}^{u_2} \cdots \sum_{z_j=0}^{u_j} C_k(s_1, s_2, \ldots, s_j, t).$$

Otherwise $A_j(k,t) = 0$.

Proof. Let s_i be a collection of times between the first step and the last step t with the property that

$$t > s_j > s_{j-1} > \cdots > s_1 \geq 1.$$

By the fundamental theorem of counting (the multiplicative rule), the number of walks that start at k and are at the border $m+1$ at the times s_i and t that avoid the boundary 0 at any step is

$$C_k(s_1, s_2, \ldots, s_j, t) := S_k(s_1) \cdot Z(s_2 - s_1) \cdot Z(s_3 - s_2) \cdots Z(s_j - s_{j-1}) \cdot Z(t - s_j).$$

Therefore, by summing over all possible values of s_i, we have the sum associated to meeting j of the intersection properties.

Note that any walk with initial location $k \in [1, m]$ and terminal location $m+1$ must have $m+1-k$ more Rights than Lefts. Thus $t - (m+1-k)$ must be positive and even. Moreover, in between each incidence with the boundary $m+1$ there must be at least one Left. Hence if a walk is to reach the boundary $m+1$ at least j times before the final step t, then it must contain at least j Lefts. Thus

$$\frac{t - (m+1-k)}{2} \geq j.$$

Hence, for any walk that reaches the boundary at times s_i for $i \in [1, j]$, we have

$$s_1 = m + 1 - k + 2z_1 \quad \text{with} \quad u_1 := \left\lfloor \frac{t - m + 1 + k - 2j}{2} \right\rfloor \geq z_1 \geq 0$$

to ensure there are enough steps to reach the boundary $m+1$ in s_1 steps while leaving enough steps $t - s_1$ to reach the boundary $m+1$ at least an additional $j-1$ times, and for $i \in [2, j]$

$$s_i = s_{i-1} + 2 + 2z_i = m + 1 - k + 2\sum_{r=1}^{i} z_i + 2(i-1),$$

with

$$u_i := \left\lfloor \frac{t - m + 1 + k - 2j - 2\sum_{r=1}^{i-1} z_i}{2} \right\rfloor \geq z_i \geq 0$$

to ensure there are enough steps to move from the boundary $m+1$ back to the boundary $m+1$ in s_i steps while leaving enough steps $t - s_i$ to reach the boundary $m+1$ at least an additional $j-i$ times. Therefore,

$$A_j(k,t) = \sum_{z_1=0}^{u_1} \sum_{z_2=0}^{u_2} \cdots \sum_{z_j=0}^{u_j} C_k(s_1, s_2, ..., s_j, t)$$

is determined by summing over all possible intersection times (having j of the boundary conditions B_{s_i}). ■

Let $U(k,t)$ be the number of walks from k to $m+1$ in t steps that avoid the boundary 0 and whose first encounter with the boundary $m+1$ occurs at time t (avoids the boundary $m+1$ in the first $t-1$ steps). In the following theorem we apply the principle of inclusion-exclusion (see Brualdi's introductory combinatorics text, [3], for a thorough treatment) to determine the number of walks whose first encounter with the boundary $m+1$ is at time t.

Theorem 3.6. For $k \in [1, m]$, if $t - (m+1-k)$ is nonnegative and even, then

$$U(k,t) = S_k(t) + \sum_{j=1}^{\left\lfloor \frac{t-(m+1-k)}{2} \right\rfloor} (-1)^j \, A_j(k,t).$$

Otherwise $U(k,t) = 0$.

Proof. By the principle of inclusion and exclusion, the number of walks from k to $m+1$ in t steps that avoid the boundary 0 and that are not at $m+1$ at a step before t, that is they have none of the intersection properties $B_s(k,t)$ for $s < t$, is given by

$$S_k(t) + \sum_{j=1}^{\left\lfloor \frac{t-(m+1-k)}{2} \right\rfloor} (-1)^j \, A_j(k,t).$$

This completes the proof. ■

Let $L(k,t)$ be the number of walks from k to 0 in t steps that avoid the boundary $m+1$ and whose first encounter with the boundary 0 occurs at time t (avoids the boundary 0 in the first $t-1$ steps).

Theorem 3.7. For $k \in [1, m]$,

$$L(k,t) = U(m+1-k, t).$$

The proof of Theorem 3.7 is omitted since it is identical to the proof of Theorem 3.6 utilizing corollaries to Theorems 3.3, 3.4 and 3.5 for walks that avoid the boundary $m+1$ and are at the boundary 0 at the last step t.

For $k, n \in [1, m]$, let $H(k,n,t)$ be the number of walks from k to n in t steps that reach the boundary and whose first encounter with the boundary is with the boundary $m+1$.

Theorem 3.8. For $k, n \in [1, m]$, if $t - |n-k|$ is positive and even, then

$$H(k,n,t) = \sum_{s=m+1-k}^{t-(m+1-n)} U(k,s) \cdot W(m+1, n, t-s).$$

Otherwise $H(k, n, t) = 0$.

Proof. Any walk from k to n in t steps that reaches the boundary and whose first encounter with the boundary is at $m + 1$ encounters the boundary for the first time at time s with $s \geq m + 1 - k$ (enough steps to reach the boundary) and $t - (m + 1 - n) \geq s$ (enough steps remaining to walk to n from $m + 1$ in $t - s$ steps). By the fundamental rule of counting, the number of walks from k to n in t steps that reach the boundary and whose first encounter with the boundary is at $m + 1$ at time s is

$$U(k, s) \cdot W(m + 1, n, t - s)$$

which corresponds to the product of the number of ways to go from k to $m + 1$ in s steps that avoid the boundary 0 and whose first encounter with the boundary $m + 1$ occurs at time s and the number of ways to go from $m + 1$ to n in $t - s$ steps. Therefore, by summing over all possible first encounters with the boundary occurring at $m + 1$, we have the number of walks from k to n in t steps that reach the boundary and whose first encounter with the boundary is with the boundary $m + 1$ is given by

$$H(k, n, t) = \sum_{s=m+1-k}^{t-(m+1-n)} U(k, s) \cdot W(m + 1, n, t - s).$$

This completes the proof. ■

For $k, n \in [1, m]$, let $J(k, n, t)$ be the number of walks from k to n in t steps that reach the boundary and whose first encounter with the boundary is with the boundary 0.

Theorem 3.9. For $k, n \in [1, m]$, if $t - |n - k|$ is positive and even, then

$$J(k, n, t) = \sum_{s=k}^{t-n} L(k, s) \cdot W(0, n, t - s).$$

Otherwise $J(k, n, t) = 0$.

The proof of Theorem 3.9 is omitted since it is nearly identical to the proof of Theorem 3.8.

For $k, n \in [1, m]$, let $G(k, n, t)$ be the number of walks from k to n in t steps that avoid the boundaries 0 and $m + 1$ in the first t steps.

Theorem 3.10. For $k, n \in [1, m]$, if $t - |n - k|$ is nonnegative and even, then

$$G(k, n, t) = W(k, n, t) - H(k, n, t) - J(k, n, t).$$

Otherwise $G(k, n, t) = 0$.

Proof. If $k, n \in [1, m]$ and $t - |n - k|$ is nonnegative and even, then the number of walks from k to n is given by $W(k, n, t)$ and $H(k, n, t)$ of these walks reach the boundary and the first encounter with the boundary is with the boundary $m + 1$ and $J(k, n, t)$ of these walks reach the boundary and the first encounter with the boundary is with the boundary 0. Therefore the number of walks that avoid the boundary is given by $G = W - H - J$.

4. Closed Form Solution for Discrete Diffusion on a Segment

The closed form solution for discrete diffusion on a segment

$$u(x, t+1) = lu(x+1, t) + ru(x-1, t) \tag{4.1}$$

for $x \in [1, m]$ with absorbing boundary conditions

$$u(0, t) = 0 = u(m+1, t) \tag{4.2}$$

and initial condition (probability of being at position k initially)

$$u(k, 0) = p(k) \tag{4.3}$$

is attained by knowing how many walks there are from an initial location k to a terminal location n in t steps that avoid the boundary, that is, knowing Green's function.

Theorem 4.1. If $n \in [0, m+1]$ and t is a nonnegative integer, then the solution of the partial difference equation (4.1), (4.2), (4.3) is

$$u(n, t) = \sum_{k=1}^{m} G(k, n, t) l^{\frac{t-(n-k)}{2}} r^{\frac{t+(n-k)}{2}} p(k).$$

Proof. If $k, n \in [1, m]$ and $t - |n - k|$ is nonnegative and even, then the number of distinct walks from k to n is given by

$$G(k, n, t)$$

and by the multiplicative rule of probability (each step is independent of the previous steps), each of these (distinct) walks has probability

$$l^{\frac{t-(n-k)}{2}} r^{\frac{t+(n-k)}{2}} p(k)$$

since each of these walks has

$$\frac{t-(n-k)}{2} \text{ Lefts, and } \frac{t+(n-k)}{2} \text{ Rights}$$

and the probability of initially starting at location k is given by

$$p(k).$$

Therefore, by summing over all possible initial locations,

$$u(n, t) = \sum_{k=1}^{m} G(k, n, t) l^{\frac{t-(n-k)}{2}} r^{\frac{t+(n-k)}{2}} p(k).$$

This completes the proof. ∎

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