First Visit Lattice Walks

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Consider the set of all possible walks of a given length that start at point $\vec{r_1}$ and end at point $\vec{r_2}$ in a lattice. There will be some subset of these walks that reach $\vec{r_2}$ for the first time only at the end of the walk. I will call this subset of walks, the first visit lattice walks. In what follows I will show that the generating function for the number of these first visit walks is related to the generating function for the total number of walks in a very simple manner. This means that if a formula for the total number of walks is known, then it is, in principle, possible to get a formula for the number of first visit walks.

First some notation: for walks of length n that start at $\vec{r_1}$ and end at $\vec{r_2}$, let $N_n(\vec{r_1}, \vec{r_2})$ be the total number of such walks and let $F_n(\vec{r_1}, \vec{r_2})$ be the number of first visit walks. Now it is clear that a lattice walk of length n from $\vec{r_1}$ to $\vec{r_2}$ will visit $\vec{r_2}$ for the first time at some step $m \leq n$ and it will then have to return to $\vec{r_2}$ after $n - m$ additional steps. The total number of ways that this can happen is

$$F_m(\vec{r_1}, \vec{r_2}) N_{n-m}(\vec{r_2}, \vec{r_2}) \tag{1}$$

Taking all possible values of m into account, means we can write $N_n(\vec{r_1}, \vec{r_2})$ as

$$N_n(\vec{r_1}, \vec{r_2}) = \delta_{\vec{r_1}, \vec{r_2}} \delta_{n,0} + \sum_{m \leq n} F_m(\vec{r_1}, \vec{r_2}) N_{n-m}(\vec{r_2}, \vec{r_2}) \tag{2}$$

where the first term accounts for the case where $\vec{r_1} = \vec{r_2}$ and $n = 0$, i.e. the number of ways of not going anywhere is 1. This expression can be inverted to get $F_n(\vec{r_1}, \vec{r_2})$ from $N_n(\vec{r_1}, \vec{r_2})$ by the use of generating functions. The generating functions for $N_n(\vec{r_1}, \vec{r_2})$ and $F_n(\vec{r_1}, \vec{r_2})$ are formal power series defined as follows:

$$N(\vec{r_1}, \vec{r_2}, z) = \sum_{n \geq 0} N_n(\vec{r_1}, \vec{r_2}) z^n \tag{3}$$

$$F(\vec{r_1}, \vec{r_2}, z) = \sum_{n \geq 0} F_n(\vec{r_1}, \vec{r_2}) z^n \tag{4}$$

Now multiplying eq.2 by z^n and summing over all n gets us

$$\sum_{n \geq 0} N_n(\vec{r_1}, \vec{r_2}) z^n = \delta_{\vec{r_1}, \vec{r_2}} + \sum_{n \geq 0} \sum_{m \leq n} F_m(\vec{r_1}, \vec{r_2}) N_{n-m}(\vec{r_2}, \vec{r_2}) z^n \tag{5}$$

The order of the double summation can be reversed to give

$$\sum_{m\geq 0}\sum_{n\geq m} F_m(\vec{r_1},\vec{r_2})N_{n-m}(\vec{r_2},\vec{r_2})z^n \tag{6}$$

Now make the change in variable $k = n - m$ to get

$$\sum_{m\geq 0}\sum_{k\geq 0} F_m(\vec{r_1},\vec{r_2})N_k(\vec{r_2},\vec{r_2})z^{m+k} \tag{7}$$

which can be written as

$$\sum_{m\geq 0} F_m(\vec{r_1},\vec{r_2})z^m \sum_{k\geq 0} N_k(\vec{r_2},\vec{r_2})z^k = F(\vec{r_1},\vec{r_2},z)N(\vec{r_2},\vec{r_2},z) \tag{8}$$

This means that eq.5 is equivalent to:

$$N(\vec{r_1},\vec{r_2},z) = \delta_{\vec{r_1},\vec{r_2}} + F(\vec{r_1},\vec{r_2},z)N(\vec{r_2},\vec{r_2},z) \tag{9}$$

Solving this equation for $F(\vec{r_1},\vec{r_2},z)$ gives:

$$F(\vec{r_1},\vec{r_2},z) = \begin{cases} \frac{N(\vec{r_1},\vec{r_2},z)}{N(\vec{r_2},\vec{r_2},z)} & \vec{r_1} \neq \vec{r_2} \\ 1 - \frac{1}{N(\vec{r_2},\vec{r_2},z)} & \vec{r_1} = \vec{r_2} \end{cases} \tag{10}$$

Note that for an infinite lattice, $N_n(\vec{r_2},\vec{r_2}) = N_n(\vec{r_1},\vec{r_1})$ and so $N(\vec{r_2},\vec{r_2},z) = N(\vec{r_1},\vec{r_1},z)$ but this is not neccessarily true for a finite lattice. If the right hand side of this equation can be expanded in powers of z then it should be possible to get a formula for $F_n(\vec{r_1},\vec{r_2})$. Now for some examples.