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Self-Avoiding Walks and Fibonacci Numbers

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ABSTRACT

By combinatorial arguments, we prove that the number of self-avoiding walks on the strip $\{0,1\} \times \mathbb{Z}$ is $8F_n - 4$ when n is odd and is $8F_n - n$ when n is even. Also, when backwards moves are prohibited, we derive simple expressions for the number of length n self-avoiding walks on $\{0,1\} \times \mathbb{Z}$, $\mathbb{Z} \times \mathbb{Z}$, the triangular lattice, and the cubic lattice.

1. INTRODUCTION

A self-avoiding walk is a path on a lattice that does not visit the same point twice. Although the number of self-avoiding walks of a prescribed length on the integer lattice $\mathbb{Z} \times \mathbb{Z}$ remains a wide open question [2], Doron Zeilberger [4] proved

Theorem 1: *For $n > 1$, the number of self-avoiding walks on the lattice* strip $\{0,1\} \times \mathbb{Z}$ *is*

$$8F_n - \varepsilon_n$$

where $\varepsilon_n = 4$, when n is odd, and $\varepsilon_n = n$ when n is even.

Zeilberger's proof uses generating functions and the appearance of Fibonacci numbers is considered a happy algebraic coincidence. Here we present an elementary combinatorial proof of this fact where the Fibonacci numbers arise in a very natural way.

2. SELF-AVOIDING WALKS ON $\{0,1\} \times \mathbb{Z}$

On the strip $\{0,1\} \times \mathbb{Z}$, a self-avoiding walk begins at the origin $(0,0)$ and at any point is allowed to move in any of three directions: up, sideways, or down, provided that we do not visit any previously visited point. Letting W_n denote the set of n-step self-avoiding walks (henceforth abbreviated as n-saws) we may describe its elements by a length n string of letters from the set $\{u, s, d\}$. For example, a typical element of W_{20} would be $dddsuuuuusuusuuuusdd$, abbreviated $d^3su^5su^2su^4sd^2$, which begins by going down 3 steps to the point $(0,-3)$, moving sideways to the point $(1,-3)$, then moving 5 steps up, and so on until finally ending at the point $(0,6)$. Letting w_n denote the number of n-saws, we can verify that $w_1 = 3$, $w_2 = 6$, $w_3 = 12$, $w_4 = 20$. Our challenge will be to explain why $w_n = 8F_n - \varepsilon_n$, by elementary combinatorial considerations.

It is well known [1] that for $n \geq 0$, F_n counts sequences of 1s and 2s that sum to $n-1$. For $k \geq 0$, let $\mathcal{F}_k$ denote the set of sequences of 1s and 2s that sum to k. Thus $\mathcal{F}_{n-1}$ has F_n elements. Our strategy is to show how almost every X in $\mathcal{F}_{n-1}$ can be used to generate eight distinct elements of W_n and that every element of W_n can be obtained uniquely in this manner. The "almost" accounts for the fact that some elements of $\mathcal{F}_{n-1}$ (two of them when n is odd, and $n/2$ of them when n is even) only generate six elements of W_n, and this explains the "error term" ε_n.

From a typical element X of $\mathcal{F}_{n-1}$, we will first generate four n-saws that end *on or above* the x-axis. We shall denote these n-saws by $SAW_1(X)$, $SAW_2(X)$, $SAW_3(X)$, $SAW_4(X)$. The horizontal reflection of these walks will produce four more n-saws that end below the x-axis. Notice that when $n > 0$ is even, there are no n-saws that end on the x-axis, and when $n > 1$ is odd, there are only two n-saws that end on the x-axis, namely $d^{(n-1)/2}su^{(n-1)/2}$ (which we call the n-cup), and its upside-down reflection $u^{(n-1)/2}sd^{(n-1)/2}$ (called the n-cap). By our construction, we will say that $SAW_1(X)$ has type (u, u) to indicate that its first and last step are in the up direction. $SAW_2(X)$ will have type (sd, u) indicating that its first step is sideways or down, and its last step is up. Similarly, SAW_3 will have type (u, sd) and $SAW_4(X)$ will have type (sd, sd).

Our primary tool for creating self-avoiding walks from sequences of 1s and 2s is the following set of instructions. For Y in $\mathcal{F}_k$ define $I(Y)$ by the rules

$$1 \to u \qquad\qquad 2 \to su.$$

That is, reading Y from left to right, every 1 tells the walk to move up and every 2 tells the walk to move sideways then up. Notice that $I(Y)$ takes exactly k steps and, if $k > 0$, will end with an up step. For example, from the sequence $Y = 2211112$ in $\mathcal{F}_{10}$, $I(Y)$ consists of the 10 steps $(su)(su)uuuu(su)$.

For X in $\mathcal{F}_{n-1}$, we define

$$SAW_1(X) = uI(X).$$

That is, $SAW_1(X)$ begins by taking one step up and then follows the instructions of X. Thus for $X_0 = 22112$ in $\mathcal{F}_8$, $SAW_1(X_0)$ is the 9-saw $uI(22112) = u\ (su)(su)uu(su)$. Notice that $SAW_1(X)$ is of type (u, u) since it begins and ends with an up step, and that every n-saw of type (u, u) ending above the x-axis can be created uniquely in this manner. Notice that when creating an n-saw from X in $\mathcal{F}_{n-1}$, we must somehow "add one step" so it achieves a length of n.

Since $SAW_2(X)$ is prescribed to be of type (sd, u), it must begin with a side or down move, and end with an up move, ending above the x-axis. Here we let the number of 2s at the beginning of X determine how many down steps to make before making a side move and then returning to the x-axis. Suppose X begins with exactly j 2s ($j \geq 0$) followed by 1 followed by a (possibly empty) string Y from $\mathcal{F}_{n-2-2j}$, then for $X = 2^j 1Y$, we define

$$SAW_2(X) = d^j su^{j+1} I(Y),$$

moving j steps down, followed by a side move, followed by $j+1$ steps up, then following the instructions of Y. For example, if $X_0 = 22112$, then $SAW_2(X_0) = d^2 su^3 I(12) = ddsuuu\, u(su)$. If $X_1 = 12221$, beginning with 1, then $SAW_2(X) = d^0 su^1 I(2221) = su\ (su)(su)(su)u$ begins with a side move. Notice that $d^j su^{j+1}$ brings us to the point $(1, 1)$ so $SAW_2(X)$ is a self-avoiding walk of type (sd, u), and it has length n because the string $2^j 1$, which has sum $2j+1$, generates the $2j+2$ steps $d^j su^{j+1}$. Finally, if X^* consists of all 2s, i.e., when n is odd and $X^* = 2^{(n-1)/2}$, then we define $SAW_2(X^*) = d^{(n-1)/2} su^{(n-1)/2}$, the n-cup.

For $SAW_3(X)$, suppose X ends with exactly j 2s, where $j \geq 0$. For $X = Y12^j$,

$$SAW_3(X) = uI(Y)u^j sd^j,$$

which is an n-saw of type (u, sd). For example, $X_0 = 22112$ maps to $SAW_3(X_0) = uI(221)u^1sd^1 = u\ (su)(su)u\ usd$. For $X^* = 2^{(n-1)/2}$ (when n is odd), we define $SAW_3(X^*) = u^{(n-1)/2}sd^{(n-1)/2}$, the n-cap.

Finally, for $SAW_4(X)$, we combine the ideas of SAW_2 and SAW_3. Suppose X begins with j 2s and ends with k 2s, where $j, k \geq 0$, and has at least two 1s in between. Then for $X = 2^j1Y12^k$,

$$SAW_4(X) = d^jsu^{j+1}I(Y)u^ksd^k,$$

is an n-saw of type (sd, sd) that begins with j down steps and ends with k down steps. For example, $X_0 = 22112$ maps to $SAW_4(X_0) = d^2su^3I(\emptyset)u^1sd^1 = ddsuuu\ usd$. If X does not have at least two 1s, then $SAW_4(X)$ is undefined. Thus when n is odd, $SAW_4(X)$ is undefined only for $X^* = 2^{(n-1)/2}$. When n is even, $SAW_4(X)$ is undefined for $\frac{n}{2}$ inputs of the form $2^j12^{\frac{(n-2)}{2}-j}$ where $0 \leq j \leq (n-2)/2$.

Summarizing, when n is odd, for every X in $\mathcal{F}_{n-1}$ (which has F_n elements), we generate four n-saws, except for the single input X^* which generates only three of them. Altogether, there are $4F_n - 1$ n-saws that end on or above the x-axis. Reflecting these (except for the n-cup and the n-cap) gives $4F_n - 3$ n-saws that end strictly below the x-axis. Altogether, there are $8F_n - 4$ n-saws as was to be shown.

When n is even, then every X in $\mathcal{F}_{n-1}$ generates four n-saws, except for the $\frac{n}{2}$ inputs of the form $2^j12^{\frac{(n-2)}{2}-j}$, which generate only three of them. Altogether, there are $4F_n - \frac{n}{2}$ n-saws, all of which end (strictly) above the x-axis. Upon reflection, we have a total of $8F_n - n$ self-avoiding walks of length n, as promised.

3. SELF-AVOIDING WALKS THAT "NEVER LOOK BACK"

In this section, we consider self-avoiding walk problems where we no longer have the option of moving in the "down" direction. These were the objects of study by Lauren Williams [3]. Using Zeilberger's generating function approach, she derived simple closed forms for counting n-step "up-side self-avoiding walks" (which we denote by n-ussaws) on various lattices. In this section, we derive many of these results by direct combinatorial arguments, beginning with the lattice strip.

Corollary 2: *For $n \geq 0$, the number of n-step up-side self-avoiding walks on the lattice strip $\{0, 1\} \times \mathbb{Z}$ is the Fibonacci number F_{n+2}.*

Proof: All n-ussaws can be uniquely obtained from X in $\mathcal{F}_{n+1}$ (which has size F_{n+2}), by taking $I(X)$ and removing the final up step. Alternatively, one can prove this by induction. Letting u_n denote the number of n-ussaws, one sees by inspection that $u_1 = 2 = F_3$, $u_2 = 3 = F_4$, and for $n \geq 3$, the last step is either up (preceded by an $(n-1)$-ussaw) or sideways, preceded by up (preceded by an $(n-2)$-ussaw); thus $u_n = u_{n-1} + u_{n-2} = F_{n+1} + F_n = F_{n+2}$, as desired. □

For other lattices, it is easy to show that the number of n-ussaws can be described by linear recurrences. Let a_n denote the number of n-ussaws on the plane $\mathbb{Z} \times \mathbb{Z}$. Let t_n denote the number of n-ussaws on the triangular lattice, where at any point in the lattice there are four legal directions: left, right, upper left, and upper right, denoted by ℓ, r, u_ℓ, u_r, respectively. Let c_n denote the number of n-ussaws on the restricted cubic lattice with points (x, y, z) where x and y are restricted to the set $\{0, 1\}$, but z may be any nonnegative integer.

Theorem 3: a) For $n \geq 2$, $a_n = 2a_{n-1} + a_{n-2}$, where $a_0 = 1$, $a_1 = 3$.

b) For $n \geq 2$, $t_n = 3t_{n-1} + 2t_{n-2}$, where $t_0 = 1$, $t_1 = 4$.
c) For $n \geq 4$, $c_n = c_{n-1} + 2c_{n-2} + 2c_{n-3} + 2c_{n-4}$, where $c_0 = 1$, $c_1 = 3$, $c_2 = 7$, $c_3 = 17$.

Proof: All of the initial conditions can be verified directly. The recurrences are all established by considering how the n-ussaw ends.
a) On the plane, every n-ussaw either ends with u^2 or it does not. For $n \geq 2$, there are a_{n-2} n-ussaws that end with u^2 (since any $(n-2)$-ussaw can have a u^2 safely appended to it) and for any $(n-1)$-ussaw, regardless of how it ends (with up, left, or right), there are two ways to legally extend it by one step so that it does not end in u^2.
b) Similarly, an n-ussaw on the triangular lattice can end with u_ℓ^2 or u_r^2 in $2t_{n-2}$ ways. Otherwise, for any $(n-1)$-ussaw, regardless of how it ends, there are three ways to legally extend it by one step so that it does not end with u_ℓ^2 or u_r^2.
c) Letting c denote a clockwise move, and d denote a counter-clockwise move, then for $n \geq 4$, an n-ussaw must either end in u, uc, ud, uc^2, ud^2, uc^3, ud^3, preceded by a ussaw of the appropriate length. □

Finally, we let $a_{n,m}$, $t_{n,m}$, $w_{n,m}$, and $c_{n,m}$ count the n-ussaws that end at a specified *height* m for the plane, the triangular lattice, the strip $\{0,1\} \times \mathbb{Z}$, and the cubic lattice, respectively.

Theorem 4: *For* $0 \leq m \leq n$,
a) $a_{n,m} = \sum_{k=0}^{m+1} \binom{m+1}{k}\binom{n-k}{m}$.
b) $t_{n,m} = 2^m a_{n,m}$.
c) $w_{n,m} = \binom{m+1}{n-m}$.
d) $\sum_{n \geq m} w_{n,m} = 2^{m+1}$.
e) $\sum_{n \geq m} c_{n,m} = 7^{m+1}$.

Proof: a) An n-ussaw of height m consists of m up steps and $n-m$ steps to the left or right. Formally, we can denote such a walk by

$$W = s_0^{j_0} u s_1^{j_1} u s_2^{j_2} u \ldots u s_{m-1}^{j_{m-1}} u s_m^{j_m},$$

where for $0 \leq i \leq m$, s_i is either equal to ℓ (denoting a left move) or equal to r (denoting a right move), $j_i \geq 0$, and $j_0 + j_1 + \cdots + j_m = n - m$. Now we ask, for $0 \leq k \leq m+1$, how many of these have exactly k of the s_i equal to ℓ with $j_i \geq 1$? In other words, how many of these walks have exactly k "left strings"? There are $\binom{m+1}{k}$ ways to choose which of the s_i will equal ℓ. Then we must count the ways to solve $j_0 + j_1 + \cdots + j_m = n - m$ where $j_i \geq 1$ when $s_i = \ell$ and $j_i \geq 0$ when $s_i = r$. Equivalently, we must count all nonnegative integer solutions to $x_0 + x_1 + \cdots + x_m = n - m - k$, whose well-known solution is $\binom{m+(n-m-k)}{n-m-k} = \binom{n-k}{m}$. Summing over all possible values of k gives us the desired solution.
b) On the triangular lattice, an n-ussaw of height m can be described as

$$s_0^{j_0} u_1 s_1^{j_1} u_2 s_2^{j_2} u_3 \ldots u_{m-1} s_{m-1}^{j_{m-1}} u_m s_m^{j_m}.$$

The same conditions apply to s_i and j_i as on the plane, but now each u_i can be designated as either u_ℓ or u_r. Hence there are 2^m times as many solutions on the triangular lattice.
c) For the lattice strip, all n-ussaws of height m are of the form

$$s^{j_0} u s^{j_1} u s^{j_2} u \ldots u s^{j_{m-1}} u s^{j_m},$$

where for $0 \le i \le m$, where each s represents a sideways move, each j_i equals 0 or 1, and $j_0 + \cdots + j_m = n - m$. Thus there are $\binom{m+1}{n-m}$ ways to choose which j_i are equal to 1.
d) One could just sum the answer to part c) to obtain

$$\binom{m+1}{0} + \binom{m+1}{1} + \cdots + \binom{m+1}{m+1} = 2^{m+1},$$

but a more combinatorially pleasing solution is to note that any ussaw of height m can be uniquely obtained from a sequence X of $m+1$ 1s and 2s by following the instructions of $I(X)$ and removing the last step. Notice that $I(X)$ is a ussaw of height $m+1$ that ends with an up step, so removing that last step gives us a ussaw of height m.
e) Letting c denote a clockwise move and d denote a counterclockwise move, all ussaws of height m on the cubic graph are of the form

$$s_0 u s_1 u s_2 u \ldots u s_m,$$

where each s_i has seven possibilities, either c, c^2, c^3, d, d^2, d^3 or "empty". More specifically, and by the same logic, $c_{n,m}$ is the coefficient of x^n of the polynomial $(1 + 2x + 2x^2 + 2x^3)^{m+1}$. □

REFERENCES

[1] A. T. Benjamin and J. J. Quinn. *Proofs That Really Count: The Art of Combinatorial Proof*, Washington DC: Mathematical Association of America, 2003.
[2] N. Madras and G. Slade. *The Self-Avoiding Walk*, Woodbine: Birkhäuser Boston, 1993.
[3] L. K. Williams. "Enumerating Up-Side Self-Avoiding Walks on Integer Lattices." *Electronic Journal of Combinatorics* **3 #R31** (1996): 1-12.
[4] D. Zeilberger. "Self-Avoiding Walks, the Language of Science, and Fibonacci Numbers." *J. Stat. Planning and Inference* **54** (1996): 135-138.

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