

A short walk can be beautiful

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Jonathan M. Borwein¹

¹CARMA, University of Newcastle

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Abstract

The story I tell is of research undertaken, with students and colleagues, in the last six or so years on short random walks. As the research progressed, my criteria for ‘beauty’ changed. Things seemingly remarkable became ‘simple’ and other seemingly simple things became more remarkable as our analytic and computational tools were refined, and understanding improved. I intentionally display some rather advanced mathematics as it is my contention – as with classical music – that one can learn to appreciate and enjoy complex formulas without needing to understand them deeply.

1 Introduction

Mathematics, rightly viewed, possesses not only truth, but supreme beauty—a beauty cold and austere, like that of sculpture, without appeal to any part of our weaker nature, without the gorgeous trappings of painting or music, yet sublimely pure, and capable of a stern perfection such as only the greatest art can show [21]. – Bertrand Russell (1872-1970)

Beauty in mathematics is frequently discussed and rarely captured precisely. Terms like ‘economy’, ‘elegance’, and ‘unexpectedness’, abound but for the most part a research mathematician will say “I know it when I see it” as with US Supreme Court Justice Potter Stewart’s famous 1964 observation on pornography [4, p. 1].

As Bertrand Russell writes mathematics is the most austere and least accessible of the arts. No one alive understands more than a small fraction of the ever growing corpus. A century ago von Neumann is supposed to have claimed familiarity with a quarter of the subject. A peek at Tim Gowers’ *Companion to Pure Mathematics* will show how impossible that now is. Clearly — except pictorially — one can only find beautiful what one can in some sense apprehend. I am a pretty broadly trained and experienced researcher, but large swathes of modern algebraic geometry or non commutative topology are too far from my ken for me to ever find them beautiful.

Aesthetics also change and old questions often become both unfashionable and seemingly arid (useless and/or ugly) — often because progress becomes too difficult as Felix Klein wrote over a

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century ago about elliptic functions [5, Preface, p. vii]. Modern mathematical computation packages like *Maple* and *Mathematica* or the open source SAGE have made it possible to go further. This is both exciting and unexpected in that we tend to view century-old well studied topics as large barren. But the new tools are game changers. This is a topic we follow up on in [15].

1.1 Background

When the facts change, I change my mind. What do you do, sir? – John Maynard Keynes (1883-1946)¹

An n -step uniform random walk in \mathbb{R}^d starts at the origin and takes n independent steps of length 1, each taken in a uniformly random direction. Thence, each step corresponds to a random vector uniformly distributed on the unit sphere. The study of such walks originates with Pearson [17], whose interest was in planar walks, which he looked at [18] as migrations of, for instance, mosquitos moving a step after each breeding cycle. Random walks in three dimensions (‘random flights’) seem first to have been studied in extenso by Rayleigh [19], and higher dimensions were mentioned in [25, §13.48].

Self-avoiding random walks are now much in vogue as they model polymers and much else. While for both random walks and their self-avoiding cousins, it is often the case that we should like to allow variable step lengths, it is only for two or three steps that we can give a closed form to the general density [25]. Thence, as often in mathematics we simplify, and in simplifying hope that we also abstract, refine, and enhance.

While we tend to think of classical areas as somehow fully understood, the truth is that we move on because, as Klein said, progress becomes too difficult. Not necessarily because there is nothing important left to say. New tools like new theorems can change the playing field and it is important that we teach such flexibility as suggested by Keynes.

Here I describe a small part of work in [6, 8] and [9], which studied analytic and number theoretic behaviour of short uniform random walks in the plane (five steps or less). In [7] we revisited the issues in higher dimensions. To our surprise (pleasure), in [7] we could provide complete extensions for most of the central results in the culminating paper [9]. Herein the underlying mathematics is taken nearly verbatim from [7] so that the interested reader finds it easy to pursue the subject in moderate.

Throughout n and d will denote the number of steps and the dimension of the random walk we are considering. Moreover, we denote by ν the half-integer

$$\nu = \frac{d}{2} - 1. \tag{1}$$

Most results are more naturally expressed in terms ν , and so we denote, for instance, by $p_n(\nu; x)$ the probability density function of the distance to the origin after n random unit steps in \mathbb{R}^d . We first develop basic Bessel integral representations for these densities beginning with Theorem 2.1. In Section 3, we turn to general results on the associated moment functions

$$W_n(\nu; s) := \int_0^\infty x^s p_n(\nu; x) dx. \tag{2}$$

In particular, we derive in Theorem 3.2 a formula for the even moments $W_n(\nu; 2k)$ as a multiple sum over the product of multinomial coefficients.

¹Quoted in “Keynes, the Man”, *The Economist*, December 18 1996, page 47.

As a consequence, we observe another interpretation of the ubiquitous Catalan numbers as the even moments of the distance after two random steps in four dimensions, and realize, more generally, in Example 3.5 the moments in four dimensions in terms of powers of the Narayana triangular matrix. We shall see that dimensions two and four are privileged in that all even moments are integral only in those two dimensions.

In Section 4 and 5 we focus on three and four step moments respectively while discussing the five-step density in Section 6 as an illustration of finding beauty in less trammelled places. We keep our notation consistent with [6, 8], and especially [9], to which we refer for details of how to exploit the Mellin transform and similar matters. We do recall that the general *hypergeometric function*— is given by

$${}_pF_q \left(\begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_q \end{matrix} \middle| x \right) := \sum_{n=0}^{\infty} \frac{(a_1)_n \dots (a_p)_n}{(b_1)_n \dots (b_q)_n} \frac{x^n}{n!}$$

and its analytic continuations. Here $(c)_n := c(c+1)\dots(c+n-1)$ is the *rising factorial*.

The hypergeometric functions and the Bessel functions defined below are two of the most significant classes of the *special functions of mathematical physics* [11]. They are special in that they are not *elementary* but are very important – and arise as solutions of second order algebraic differential equations. They are ubiquitous in our mathematical description of the physical universe. Like precious stones each has its own best features and occasional flaws.

2 The probability density

Old questions are solved by disappearing, evaporating, while new questions corresponding to the changed attitude of endeavor and preference take their place. Doubtless the greatest dissolvent in contemporary thought of old questions, the greatest precipitant of new methods, new intentions, new problems, is the one effected by the scientific revolution that found its climax in the “Origin of Species.” [10, pp. 1–19] – John Dewey (1859-1952)

We summarize from [13, Chapter 2.2] how to write the probability density $p_n(\nu; x)$ of an n -step random walk in d dimensions. Throughout, the *normalized Bessel function of the first kind* is

$$j_\nu(x) = \nu! \left(\frac{2}{x} \right)^\nu J_\nu(x) = \nu! \sum_{m \geq 0} \frac{(-x^2/4)^m}{m!(m+\nu)!}. \quad (3)$$

With this normalization we have $j_\nu(0) = 1$ and

$$j_\nu(x) \sim \frac{\nu!}{\sqrt{\pi}} \left(\frac{2}{x} \right)^{\nu+1/2} \cos \left(x - \frac{\pi}{2} \left(\nu + \frac{1}{2} \right) \right) \quad (4)$$

as $x \rightarrow \infty$ on the real line. The Bessel function is a natural generalization of the exponential: $j_0(2\sqrt{x}) = \sum_{n \geq 0} x^n/n!^2$ while $\exp(x) = \sum_{n \geq 0} x^n/n!$. Note also that $j_{1/2}(x) = \text{sinc}(x) = \sin(x)/x$, which in part explains why analysis in 3-space is so simple. More generally, all half-integer order $j_\nu(x)$ are elementary and so the odd dimensional theory is much simpler. While only two and three dimensions arise easily in physically meaningful settings, we have discovered that four and higher dimensional information is needed to explain two dimensional behaviour. This elegant discovery is reminiscent of how one needs complex numbers to understand real polynomials.

Theorem 2.1. (Bessel integrals for the densities) *The probability density function of the distance to the origin in $d \geq 2(\nu \geq 0)$ dimensions after $n \geq 2$ steps is, for $x > 0$,*

$$p_n(\nu; x) = \frac{2^{-\nu}}{\nu!} \int_0^\infty (tx)^{\nu+1} J_\nu(tx) j_\nu^n(t) dt. \quad (5)$$

More generally, for integer $k \geq 0$, and $x > 0$,

$$p_n(\nu; x) = \frac{2^{-\nu}}{\nu!} \frac{1}{x^{2k}} \int_0^\infty (tx)^{\nu+k+1} J_{\nu+k}(tx) \left(-\frac{1}{t} \frac{d}{dt}\right)^k j_\nu^n(t) dt. \quad (6)$$

We shall see that (6) is more tractable. It is also computationally useful.

The densities $p_3(\nu; x)$ in dimensions 2, 3, ..., 9 are shown to the left in Figure 1. In the plane, there is a logarithmic singularity at $x = 1$, otherwise the functions are at least continuous in the interval of support $[0, 3]$. The densities of four-step walks are shown on the right of Figure 1, and corresponding plots for five steps are shown in Figure 4. These simple pictures are only easy to draw given a good implementation of the Bessel function and reasonable plotting software! The striking 4-step planar density has been named “the shark-fin curve” by the late Richard Crandall. This naming itself is a subversive aesthetic act — after attaching the name one can never look at the graph in the same way again — as is discussed in John Berger’s seminal 1972 TV series and subsequent book “Ways of Seeing” http://en.wikipedia.org/wiki/Ways_of_Seeing.

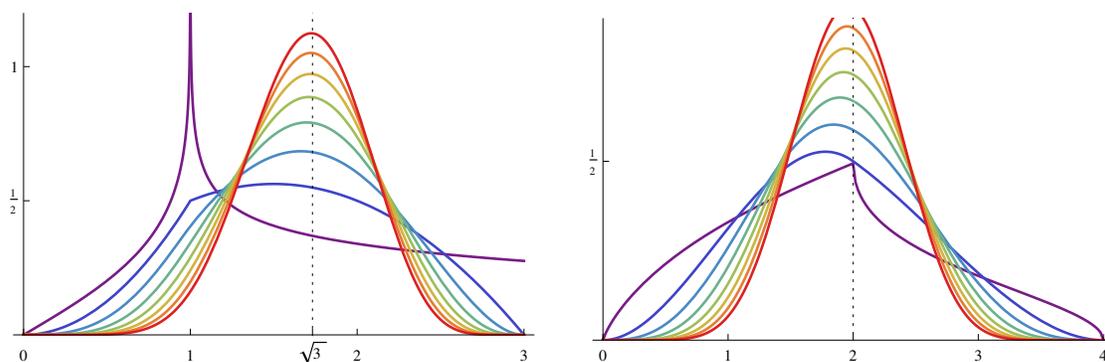


Figure 1: $p_3(\nu; x)$ and $p_4(\nu; x)$ for $\nu = 0, \frac{1}{2}, 1, \dots, \frac{7}{2}$

Observe how the densities center and spike as the dimension increases. This is a general phenomenon: $p_n(\nu; x)$ approaches a Dirac distribution centered at \sqrt{n} . The intuition is that as the dimension increases, the directions of the steps increasingly tend to be close to orthogonal. Pythagoras’ theorem therefore predicts the distance after n steps is about \sqrt{n} .

Integrating (5), yields a Bessel integral representation for the cumulative distribution functions,

$$P_n(\nu; x) = \int_0^x p_n(\nu; y) dy, \quad (7)$$

of the distance to the origin after n steps in d dimensions.

Corollary 2.2. (Cumulative distribution) Suppose $d \geq 2$ and $n \geq 2$. Then, for $x > 0$,

$$P_n(\nu; x) = \frac{2^{-\nu}}{\nu!} \int_0^\infty (tx)^{\nu+1} J_{\nu+1}(tx) j_\nu^n(t) \frac{dt}{t}. \quad (8)$$

So we see that the Bessel function is not just computationally necessary but it is also theoretically unavoidable. Just as the *Airy* function is needed to understand rainbows [11], these functions are often the preferred way to capture the natural universe.

Example 2.3. (Kluyver's Theorem) A justifiably famous result of Kluyver [14] is that,

$$P_n(0; 1) = \frac{1}{n+1}, \quad (9)$$

for $n \geq 2$. That is, after n unit steps in the plane, the probability of being within one unit of home is $1/(n+1)$. How simple, how unexpected, how beautiful! Equation (9) is almost immediate from (8) on appealing to the Fundamental theorem of calculus since $J_1 = j'_0$. Amazing! An elementary proof of this was given only recently [3]. It is natural to ask what happens in higher dimensions. We do not know in entirety, but some unexpected results follow.

(a) In the case of two steps, we have

$$P_2(\nu; x) = \frac{x^{2\nu+1}}{2\sqrt{\pi}} \frac{\Gamma(\nu+1)}{\Gamma(\nu+3/2)} {}_2F_1 \left(\begin{matrix} \frac{1}{2} + \nu, \frac{1}{2} - \nu \\ \frac{3}{2} + \nu \end{matrix} \middle| \frac{x^2}{4} \right),$$

which, in the case of integers $\nu \geq 0$ and $x = 1$, reduces to

$$P_2(\nu; 1) = \frac{1}{3} - \frac{\sqrt{3}}{4\pi} \sum_{k=0}^{\nu-1} \frac{3^k}{(2k+1) \binom{2k}{k}}. \quad (10)$$

In particular, in dimensions 4, 6 and 8,

$$P_2(1; 1) = \frac{1}{3} - \frac{\sqrt{3}}{4\pi}, \quad P_2(2; 1) = \frac{1}{3} - \frac{3\sqrt{3}}{8\pi}, \quad P_2(3; 1) = \frac{1}{3} - \frac{9\sqrt{3}}{20\pi}, \quad \dots$$

From (10) it is clear that $P_2(\nu; 1)$ is of the form $\frac{1}{3} - c_\nu \frac{\sqrt{3}}{\pi}$ for some rational $c_\nu > 0$.

(b) In the case of three steps, we find

$$P_3(1; 1) = \frac{1}{4} - \frac{4}{3\pi^2}, \quad P_3(2; 1) = \frac{1}{4} - \frac{256}{135\pi^2}, \quad P_3(3; 1) = \frac{1}{4} - \frac{2048}{945\pi^2}, \quad \dots$$

Indeed, for integers $\nu \geq 0$, we have the general formula

$$P_3(\nu; 1) = \frac{1}{4} - \frac{1}{3\pi^2} \sum_{k=0}^{\nu-1} 2^{6k} \frac{(11k+8)k!^5}{(2k+1)!(3k+2)!}. \quad (11)$$

From (11) it is clear that $P_3(\nu; 1)$ is of the form $\frac{1}{4} - c_\nu \frac{1}{\pi^2}$ for some rational $c_\nu > 0$. In each case as n goes to infinity, the probability goes to zero. This is not surprising for probabilistic reasons. For $n \geq 4$, much less is accessible [2, §5], and it would be interesting to obtain a more complete extension of Kluyver's result to higher dimensions. \diamond

3 The moment functions

To see a World in a Grain of Sand
 And a Heaven in a Wild Flower,
 Hold Infinity in the palm of your hand
 And Eternity in an hour. – William Blake (1757–1827)²

Theorem 2.1 allows us to prove a Bessel integral representation for the *moment function*

$$W_n(\nu; s) = \int_0^\infty x^s p_n(\nu; x) dx$$

of the distance to the origin after n random steps.

Theorem 3.1. (Bessel integral for the moments) *Let $n \geq 2$ and $d \geq 2$. For any $k \geq 0$,*

$$W_n(\nu; s) = \frac{2^{s-k+1} \Gamma\left(\frac{s}{2} + \nu + 1\right)}{\Gamma(\nu + 1) \Gamma\left(k - \frac{s}{2}\right)} \int_0^\infty x^{2k-s-1} \left(-\frac{1}{x} \frac{d}{dx}\right)^k j_\nu^n(x) dx, \quad (12)$$

provided that $k - n(\nu + 1/2) < s < 2k$.

In particular, for $n > 2$, the first pole of $W_n(\nu; s)$ occurs at $s = -(2\nu + 2) = -d$.

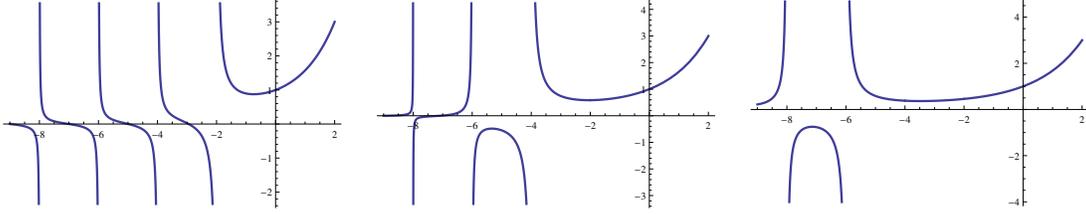


Figure 2: $W_3(\nu; s)$ on $[-9, 2]$ for $\nu = 0, 1, 2$.

We next obtain from Theorem 2.1 a summatory expression for the even moments.

Theorem 3.2. (Multinomial sum for moments) *The even moments of an n -step walk in dimension d are given by*

$$W_n(\nu; 2k) = \frac{(k + \nu)! \nu!^{n-1}}{(k + n\nu)!} \sum_{k_1 + \dots + k_n = k} \binom{k}{k_1, \dots, k_n} \binom{k + n\nu}{k_1 + \nu, \dots, k_n + \nu}.$$

Proof. Replace k by $k + 1$ in (12) and set $s = 2k$, to obtain

$$W_n(\nu; 2k) = \frac{2^k (k + \nu)!}{\nu!} \int_0^\infty -\frac{d}{dx} \left(-\frac{1}{x} \frac{d}{dx}\right)^k j_\nu^n(x) dx = \left[\frac{(k + \nu)!}{\nu!} \left(-\frac{2}{x} \frac{d}{dx}\right)^k j_\nu^n(x) \right]_{x=0}. \quad (13)$$

²Fragment from *Songs of Innocence*.

Observe that, as formal power series, we have

$$\left[\left(-\frac{2}{x} \frac{d}{dx} \right)^k \sum_{m \geq 0} a_m \left(-\frac{x^2}{4} \right)^m \right]_{x=0} = k! a_k.$$

Recall from (3) the series $j_\nu(x) = \nu! \sum_{m \geq 0} \frac{(-x^2/4)^m}{m!(m+\nu)!}$, to conclude that

$$W_n(\nu; 2k) = \frac{(k+\nu)!}{\nu!} \nu! n k! \sum_{m_1 + \dots + m_n = k} \frac{1}{m_1! \dots m_n!} \frac{1}{(m_1 + \nu)! \dots (m_n + \nu)!},$$

which is equivalent to the claimed formula. \square

Example 3.3. In the case $k = 1$, Theorem 3.2 implies that the second moment of an n -step random walk is $W_n(\nu; 2) = n$. Similarly, we find that

$$W_n(\nu; 4) = \frac{n(n(\nu+2) - 1)}{\nu+1}. \quad (14)$$

More generally, Theorem 3.2 shows $W_n(\nu; 2k)$ is a polynomial of degree k in n , with coefficients that are rational functions in ν . For instance,

$$W_n(\nu; 6) = \frac{n(n^2(\nu+2)(\nu+3) - 3n(\nu+3) + 4)}{(\nu+1)^2} \quad (15)$$

and so on. Equation (15) shows that only in two or four dimensions can all the moments be integers. \diamond

Using the explicit expression of the even moments we derive the following convolution relation.

Corollary 3.4. (Moment recursion) *For positive integers n_1, n_2 , half-integer ν and nonnegative integer k we have*

$$W_{n_1+n_2}(\nu; 2k) = \sum_{j=0}^k \binom{k}{j} \frac{(k+\nu)! \nu!}{(k-j+\nu)! (j+\nu)!} W_{n_1}(\nu; 2j) W_{n_2}(\nu; 2(k-j)). \quad (16)$$

The special case $n_2 = 1$, relates moments of an n -step walk to those of an $(n-1)$ -step walk.

Example 3.5. (Integrality of two and four dimensional even moments) Corollary 3.4 is an efficient way to compute even moments in any dimension and so to data-mine. For illustration, because they are integral, we record the moments in two and four dimensions for $n = 2, 3, \dots, 6$.

$$\begin{aligned} W_2(0; 2k) &: 1, 2, 6, 20, 70, 252, 924, 3432, 12870, \dots \\ W_3(0; 2k) &: 1, 3, 15, 93, 639, 4653, 35169, 272835, 2157759, \dots \\ W_4(0; 2k) &: 1, 4, 28, 256, 2716, 31504, 387136, 4951552, 65218204, \dots \\ W_5(0; 2k) &: 1, 5, 45, 545, 7885, 127905, 2241225, 41467725, 798562125, \dots \\ W_6(0; 2k) &: 1, 6, 66, 996, 18306, 384156, 8848236, 218040696, 5651108226, \dots \end{aligned}$$

For $n = 2$, these are central binomial coefficients, while, for $n = 3, 4$, these are Apéry-like sequences, see (26). In general they are sums of squares of multinomial coefficients and so integers.

Likewise, the initial even moments in four dimensions are as follows.

$$\begin{aligned} W_2(1; 2k) &: 1, 2, 5, 14, 42, 132, 429, 1430, 4862, \dots \\ W_3(1; 2k) &: 1, 3, 12, 57, 303, 1743, 10629, 67791, 448023, \dots \\ W_4(1; 2k) &: 1, 4, 22, 148, 1144, 9784, 90346, 885868, 9115276, \dots \\ W_5(1; 2k) &: 1, 5, 35, 305, 3105, 35505, 444225, 5970725, 85068365, \dots \\ W_6(1; 2k) &: 1, 6, 51, 546, 6906, 99156, 1573011, 27045906, 496875786, \dots \end{aligned}$$

Observe that the first three terms are as determined in Example 3.3. In the two-step case in four dimensions, we find that the even moments are the *Catalan numbers* C_k , that is

$$W_2(1; 2k) = \frac{(2k+2)!}{(k+1)!(k+2)!} = C_{k+1}, \quad C_k := \frac{1}{k+1} \binom{2k}{k}. \quad (17)$$

This adds another interpretation to the impressive array of things counted by the Catalan numbers.

In two and four dimensions *only*, all even moments are integers (compare, for instance, (14)). This is obvious for two dimensions from Theorem 3.2 which becomes

$$W_n(0; 2k) = \sum_{k_1 + \dots + k_n = k} \binom{k}{k_1, \dots, k_n}^2$$

counts *abelian squares* [20]. On the other hand, to show that $W_n(1; 2k)$ is always integral, we recursively apply (16) and note that it is known (see Example 3.6) that the factors

$$\binom{k}{j} \frac{(k+1)!}{(k-j+1)!(j+1)!} = \frac{1}{j+1} \binom{k}{j} \binom{k+1}{j} \quad (18)$$

are integers for all nonnegative j and k . The numbers (18) are known as *Narayana numbers* and occur in various counting problems; see, for instance, [24, Problem 6.36]. \diamond

Thus, integrality of the 4-dimensional moments is a deeper – and hence arguably more beautiful – fact which we first discovered numerically before being led to the Narayana triangle.

Example 3.6. (Narayana numbers and triangle) The recursion for $W_n(\nu; 2k)$ is equivalent to the following: for given ν , let $A(\nu)$ be the infinite lower triangular matrix with entries

$$A_{k,j}(\nu) = \binom{k}{j} \frac{(k+\nu)! \nu!}{(k-j+\nu)!(j+\nu)!} \quad (19)$$

for row indices $k = 0, 1, 2, \dots$ and column indices $j = 0, 1, 2, \dots$. Then the row sums of $A(\nu)^n$ are given by the moments $W_{n+1}(\nu; 2k)$, $k = 0, 1, 2, \dots$. For instance, in the case $\nu = 1$,

$$A(1) = \begin{bmatrix} 1 & 0 & 0 & 0 & \dots \\ 1 & 1 & 0 & 0 & \\ 1 & 3 & 1 & 0 & \\ 1 & 6 & 6 & 1 & \\ \vdots & & & & \ddots \end{bmatrix}, \quad A(1)^3 = \begin{bmatrix} 1 & 0 & 0 & 0 & \dots \\ 3 & 1 & 0 & 0 & \\ 12 & 9 & 1 & 0 & \\ 57 & 72 & 18 & 1 & \\ \vdots & & & & \ddots \end{bmatrix},$$

with the row sums $1, 2, 5, 14, \dots$ and $1, 4, 22, 148, \dots$ corresponding to the moments $W_2(1; 2k)$ and $W_4(1; 2k)$ as given in Example 3.5. Observe that, since the first column of $A(\nu)$ is composed of 1's, the sequence of moments $W_n(1; 2k)$ can also be directly read off from the first column of $A(\nu)^n$. The matrix $A(1)$ is known as the *Narayana triangle* or the *Catalan triangle* [23, A001263]. [The OEIS is like a mathematical bird guide. We see/hear something striking and our guide points us to the species.] \diamond

Remark 3.7 (Beauty in Complexity). As with music, aesthetic experience relies on resolving or adapting to seeming complexity. That is why most popular music can never compete with a Dvorjak symphony. It also explains why it is hard to make intrinsically simple mathematics seem as beautiful as a simple — short, elegant, transparent — resolution of harder material.

What is so beautiful in the case of the Narayana triangle, is that we can completely describe the even moments in four dimensions in terms of powers of one known combinatorial matrix and the ubiquitous Catalan numbers. We have reduced subtle probabilistic and analytic objects to their purely combinatorial roots. One of my undergraduate collaborators, Ghislain McKay, has subsequently proven lovely and elementary results regarding the divisibility properties of the moments entirely from the representation in terms of the Narayana triangle. We have also illustrated another source of beauty in mathematics. As we peel away parts of the onion we often uncover unexpected complexity in seemingly simple or unexplored settings.

Further study is rewarded by a level of simplicity yet below. We are offered a glimpse of infinity in Blake's grain of sand. I am reminded that fame or reputation in art and in mathematics can be changeable. Consider the prevailing view of William Blake — as obscure and exotic — before Northrop Frye's 1947 book *A fearful symmetry*. Consider also the impact of live piano performances by Felix Mendelssohn³ (1829) and — especially of the Goldberg Variations — by Glenn Gould (1955) on our current positive reception of Bach who died in 1750. \diamond

Recall that a function f is of *exponential type* if $|f(z)| \leq M e^{c|z|}$ for constants M and c .

Theorem 3.8. (Carlson's Theorem) *Let f be analytic in the right half-plane $\operatorname{Re} z \geq 0$ and of exponential type with the additional requirement that*

$$|f(z)| \leq M e^{d|z|}$$

for some $d < \pi$ on the imaginary axis. If $f(k) = 0$ for $k = 0, 1, 2, \dots$, then $f(z) = 0$ identically.

Above we went from the continuous to the discrete. Carlson's magisterial theorem now provides a magical way to go from the discrete to the continuous — from properties known only at natural numbers to properties holding in the complex half-plane or plane.

4 Moments of 3-step walks

The difficulty lies, not in the new ideas, but in escaping the old ones, which ramify, for those brought up as most of us have been, into every corner of our minds. — John Maynard Keynes⁴

³See <http://lcweb2.loc.gov/diglib/ahas/loc.natlib.ahas.200156436/default.html>.

⁴Quoted in K E Drexler, *Engines of Creation: The Coming Era of Nanotechnology*, New York, 1987.

Example 4.1. Applying *creative telescoping* [7] to the binomial sum for $W_3(\nu; 2k)$, we derive that the moments $W_3(\nu; 2k)$ satisfy the recursion

$$\begin{aligned} & (k + 2\nu + 1)(k + 3\nu + 1)W_3(\nu; 2k + 2) \\ &= \frac{1}{2} \left(20 \left(k + \frac{1}{2}\right)^2 + 60 \left(k + \frac{1}{2}\right) \nu + 36\nu^2 + 1 \right) W_3(\nu; 2k) - 9k(k + \nu)W_3(\nu; 2k - 2). \end{aligned} \quad (20)$$

Observe that $W_n(\nu; s)$ is analytic for $\operatorname{Re} s \geq 0$ and is bounded in that half-plane by $|W_n(\nu; s)| \leq n^{\operatorname{Re} s}$ (because, the distance after n steps is bounded by n). It therefore follows from Carlson's Theorem, see [6, Theorem 4], that (20) remains valid for all complex values of k . \diamond

The next equation

$$W_3(\nu; 2k) = {}_3F_2 \left(\begin{matrix} -k, -k - \nu, \nu + 1/2 \\ \nu + 1, 2\nu + 1 \end{matrix} \middle| 4 \right). \quad (21)$$

gives a hypergeometric expression for the even moments of a 3-step random walk. We discovered numerically that, in the plane, the *real part* of this expression still evaluates odd moments [6]. (e.g., $W_3(0; 1) = \operatorname{Re}(1.5745972 \pm 0.12602652i)$). The \pm sign depends on which branch cut is used for the hypergeometric function. These odd moments are much harder to obtain; it was first proved based on this observation, that the average distance of a planar 3-step random walk is

$$W_3(0; 1) = A + \frac{6}{\pi^2} \frac{1}{A} \approx 1.5746, \quad (22)$$

where

$$W_3(0; -1) = \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6\left(\frac{1}{3}\right) =: A. \quad (23)$$

This discovery for me felt precisely like Keats' description of "On first looking into Chapman's Homer."⁵ We then establish the transcendental nature of odd moments of 3-step walks in all even dimensions by showing they are rational linear combinations of A and $1/(\pi^2 A)$.

Theorem 4.2. (Hypergeometric form of W_3 at odd integers) *Suppose that d is even, that is, ν is an integer. For all odd integers $s \geq -2\nu - 1$,*

$$W_3(\nu; s) = \operatorname{Re} {}_3F_2 \left(\begin{matrix} -s/2, -s/2 - \nu, \nu + 1/2 \\ \nu + 1, 2\nu + 1 \end{matrix} \middle| 4 \right).$$

Example 4.3. (Odd moments $W_3(\nu; \cdot)$ in even dimensions) The planar case of Theorem 4.2 was used in [6] to prove the average distance to the origin after three steps in the plane is given by (22). It is a consequence of (20), extended to complex k , that all planar odd moments are \mathbb{Q} -linear combinations of $A = \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6(1/3)$, defined in (23), and $1/(\pi^2 A)$. A dimensional recursion used in the proof of Theorem 4.2 shows this extends to all even dimensions. For instance,

$$W_3(1; -3) = \frac{4}{3}A - \frac{4}{\pi^2} \frac{1}{A}, \quad W_3(1; -1) = \frac{4}{15}A + \frac{4}{\pi^2} \frac{1}{A}.$$

Moreover, the average distance to the origin after three random steps in four dimensions is

$$W_3(1; 1) = \frac{476}{525}A + \frac{52}{7\pi^2} \frac{1}{A} \approx 1.6524,$$

with similar evaluations in six or higher even dimensions. \diamond

⁵"Then felt I like some watcher of the skies
When a new planet swims into his ken;" see <http://www.poetryfoundation.org/poem/173746>.

Example 4.4. Theorem 4.2 fails in odd dimensions. For instance, in dimension 3,

$$W_3\left(\frac{1}{2}; s\right) = \frac{1}{4} \frac{3^{s+3} - 3}{(s+2)(s+3)}$$

while for integer $s > 0$

$${}_3F_2\left(\begin{matrix} -s/2, -s/2 - 1/2, 1 \\ 3/2, 2 \end{matrix} \middle| 4\right) = \frac{1}{4} \frac{3^{s+3} - 2 - (-1)^s}{(s+2)(s+3)}$$

only agrees for even s . This has its own beauty as it shows Carlson’s theory can not now apply even to go from even integer to integers. \diamond

Remark 4.5. (Meditation on beauty, I) The role of Carlson’s Theorem 3.8 may seem natural and beautiful, but depending on the place and the observer it may seem natural and ugly, or mysterious and beautiful, or worse. Many results in special function theory, in number theory or mathematical physics do seemingly rely on it. In a period where substantial experimental mathematics is possible, it is a wonderful and elegant tool.

We were originally introduced to the planar moments in the form

$$W_n(0; s) = \int_0^{2\pi} \int_0^{2\pi} \cdots \int_0^{2\pi} |e^{\theta_1 i} + e^{\theta_2 i} + \cdots + e^{\theta_n i}|^s d\theta_n d\cdots \theta_2 d\theta_1, \quad (24)$$

during a study of numerical multidimensional integrals. For s an even integer this can be evaluated in closed form by computer algebra. This let us to become familiar with the combinatorics of even moments in the plane, but was painful for odd integers — even for $s = 1$. Luckily Carlson’s theorem let us find and prove the core results for three step walks in the plane, such as (22) which astonished us, even before we found the lovely classical work of Kluyver. That said, many of the higher dimensional results would have been impossible from our original naive approach. We still lack an explicit ‘bijective’ combinatorial interpretation of $W_n(1; 2k)$ — largely because we have no nice 4-dimensional analogue of (24). \diamond

5 Moments of 4-step walks

Mathematics is not a careful march down a well-cleared highway, but a journey into a strange wilderness, where the explorers often get lost. Rigour should be a signal to the historian that the maps have been made, and the real explorers have gone elsewhere. [1] –W.S. (Bill) Angelin.

The tidy ex post facto beauty of a well written mathematics textbook or Bourbaki monograph is quite different from the beauty of discoveries in still wild parts of the subject.

Theorem 3.1 leads to special function representations with potential far beyond what can be learned from (24). The beautiful image⁶ in Figure 3 is a fruit of such a representation in which each point is coloured by its argument (black is zero and white infinity). Note the real poles and two complex zeros. Clearly to be able to draw this meant we were no longer in a wilderness but neither were we ready for Bourbaki. I remark that the needs of a scientific illustration to inform compete with purely aesthetic goals. For the later we might well choose a quite different colour palette.

The convolution in Corollary 3.4 leads to:

⁶To appear as August in *Complex Beauties*, 2016, see <http://www.mathe.tu-freiberg.de/fakultaet/information/math-calendar-2015>. The preceding three months illustrate the components of the construction.

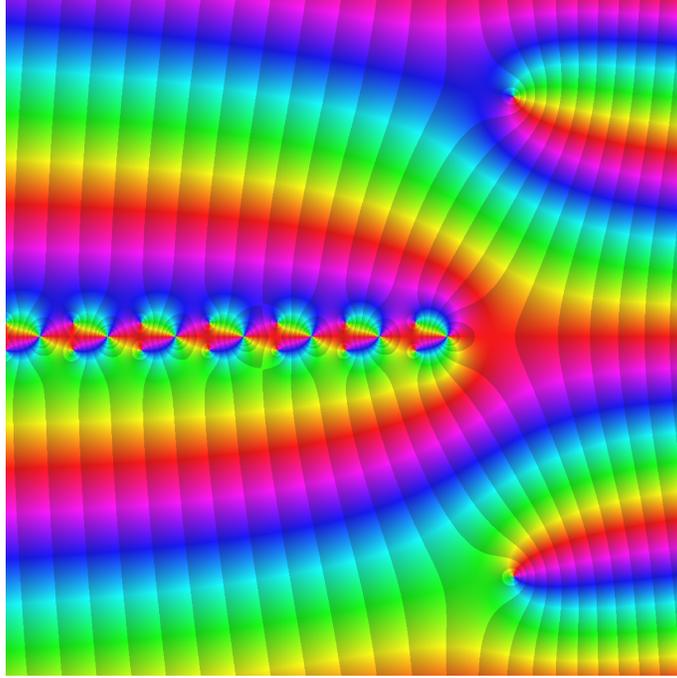


Figure 3: The moment function $W_4(0; s)$ in the complex plane.

Lemma 5.1. *The nonnegative even moments for a 4-step walk in d dimensions are*

$$W_4(\nu; 2k) = \sum_{j=0}^k \frac{\binom{k}{j} \binom{k+\nu}{j}}{\binom{j+\nu}{j}} \frac{\binom{2j+2\nu}{j}}{\binom{j+\nu}{j}} \frac{\binom{2(k-j)+2\nu}{k-j}}{\binom{k-j+\nu}{k-j}}. \quad (25)$$

Example 5.2. (Generalised Domb numbers) The binomial sums in (25) generalize the *Domb numbers*, also known as the *diamond lattice numbers* [23, A002895],

$$W_4(0; 2k) = \sum_{j=0}^k \binom{k}{j}^2 \binom{2j}{j} \binom{2(k-j)}{k-j}, \quad (26)$$

for $k = 0, 1, 2, \dots$, which play an important role in the plane. In four space, (16) with (17) yields

$$W_4(1; 2k) = \sum_{j=1}^{k+1} N(k+1, j) C_j C_{k-j+2},$$

where C_k are the Catalan numbers, as in (17), and

$$N(k+1, j+1) = \frac{1}{j+1} \binom{k}{j} \binom{k+1}{j}$$

are the Narayana numbers, as in Example 5.2. We are able to show that the generating function for $W_4(\nu; 2k)$ can be given in terms of hypergeometric functions whenever the dimension is even. \diamond

Corollary 5.3. (Hypergeometric form of W_4 at even integers) For $k = 0, 1, 2, \dots$, we have

$$W_4(\nu; 2k) = \frac{\binom{2k+2\nu}{k}}{\binom{k+\nu}{k}} {}_4F_3 \left(\begin{matrix} -k, -k-\nu, -k-2\nu, \nu+1/2 \\ \nu+1, 2\nu+1, -k-\nu+1/2 \end{matrix} \middle| 1 \right).$$

We note that this hypergeometric function is *well-poised* [11, §16.4].

Example 5.4. Applying creative telescoping to (25), we derive that the moments $W_4(\nu; 2k)$ satisfy

$$\begin{aligned} & (k+2\nu+1)(k+3\nu+1)(k+4\nu+1)W_4(\nu; 2k+2) \\ &= \left((k+\frac{1}{2})+2\nu \right) \left(20(k+\frac{1}{2})^2 + 80(k+\frac{1}{2})\nu + 48\nu^2 + 3 \right) W_4(\nu; 2k) \\ & \quad - 64k(k+\nu)(k+2\nu)W_4(\nu; 2k-2). \end{aligned} \quad (27)$$

As in Example 4.1, $W_4(\nu; s)$ is analytic, exponentially bounded for $\operatorname{Re} s \geq 0$ and bounded on vertical lines. Hence, Carlson's Theorem 3.8 again applies to shows (27) extends to complex k . \diamond

Example 5.5. (Odd moments $W_4(\nu; \cdot)$ in even dimensions) The average distance to the origin after four random steps in the plane, as well as all odd moments, can be evaluated in terms of the *complete elliptic integral* $K'(k) := \int_0^{\pi/2} \frac{d\theta}{\sqrt{1-(1-k^2)\sin^2\theta}}$, namely we set

$$\begin{aligned} A &:= \frac{1}{\pi^3} \int_0^1 K'(k)^2 dk = \frac{\pi}{16} {}_7F_6 \left(\begin{matrix} \frac{5}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{1}{4}, 1, 1, 1, 1, 1 \end{matrix} \middle| 1 \right), \\ B &:= \frac{1}{\pi^3} \int_0^1 k^2 K'(k)^2 dk = \frac{3\pi}{256} {}_7F_6 \left(\begin{matrix} \frac{7}{4}, \frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{3}{4}, 2, 2, 2, 2, 1 \end{matrix} \middle| 1 \right). \end{aligned}$$

Then, in two dimensions,

$$W_4(0; -1) = 4A, \quad W_4(0; 1) = 16A - 48B.$$

It follows from (27), extended to complex values, that odd moments are rational linear combinations of A and B . To extend this to higher dimensions, we discovered and then proved that

$$\begin{aligned} 0 &= 3(s+2)(s+6\nu)(s+8\nu)(s+8\nu-2)W_4(\nu; s) \\ & \quad + 256\nu^3(s+4\nu)W_4(\nu-1; s+2) - 8\nu^3(5s+32\nu-6)W_4(\nu-1; s+4). \end{aligned} \quad (28)$$

We can now induct on the dimension to conclude that, in any even dimension, the odd moments lie in the \mathbb{Q} -span of the constants A and B , which arose in the planar case. For instance, we find that the average distance to the origin after four random steps in four dimensions is

$$W_4(1; 1) = \frac{3334144}{165375}A - \frac{11608064}{165375}B,$$

and so on. \diamond

Remark 5.6. (Meditation on beauty, II) Bessel functions like some other special functions (e.g., the Gamma function, hypergeometric functions and elliptic integrals) are extraordinary in both their theoretical ubiquity and applicability, but because of my pure mathematics training,

I knew them only peripherally until my research moved into mathematical physics, random walk theory and other “boundary” fields. They can even be used to produce immensely complicate standing water waves, spelling out corporate names! ⁷

To me now they are a mathematical gem, every facet of which rewards further examination. To me as a student, they were only the solution to a second-order algebraic definition which I had to look up each time. Moreover, looking them up is now easy and fun thanks to sources like [11]. I could make similar remarks about combinatorial objects, such as the Catalan numbers and the Narayana triangle. In this case familiarity breeds content not contempt. Moreover, computer algebra packages make it wonderfully easy to become familiar with the objects. \diamond

6 Densities of 5-step walks

The mathematician’s patterns, like the painter’s or the poet’s must be beautiful; the ideas like the colours or the words, must fit together in a harmonious way. Beauty is the first test: there is no permanent place in the world for ugly mathematics. – G.H. Hardy (1887-1977) ⁸

Almost all mathematicians agree with Hardy until asked to put flesh on the bones of his endorsement of beauty. Beauty may be the first test but it is the eye of the beholder. Hardy, in the twelfth of his of his twelve lectures given as a eulogy for the singular Indian genius Srinivasa Ramanujan (1887–1921), described a result of Ramanujan – now viewed as one his finest – somewhat dismissively as “a remarkable formula with many parameters.” ⁹

The 5-step densities for dimensions up to 9 are shown in Figure 4. A peculiar feature in the plane is the striking (approximate) linearity on the initial interval $[0, 1]$. As Pearson [18] commented:

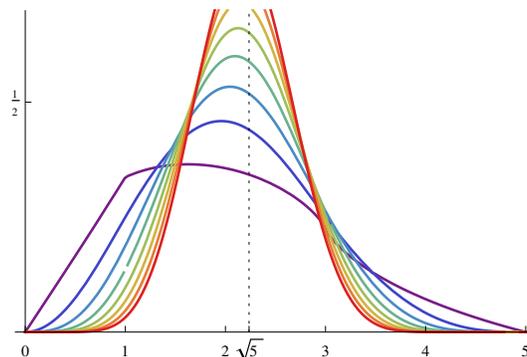


Figure 4: $p_5(\nu; x)$ for $\nu = 0, \frac{1}{2}, 1, \dots, \frac{7}{2}$

“the graphical construction, however carefully reinvestigated, did not permit of our considering the curve to be anything but a *straight* line... Even if it is not absolutely true, it exemplifies the extraordinary power of such integrals of J products [that is, (5)] to give extremely close approximations to such simple forms as horizontal lines.”

⁷See <http://www.openscience.org/blog/?p=193>. (See also Pearson’s comment in the next section.)

⁸In his delightful *A Mathematician’s Apology*, 1941.

⁹See Ole Warnaar’s 2013 contribution in “Srinivasa Ramanujan Going Strong at 125, Part II,” available at <http://www.ams.org/notices/201301/rnoti-p10.pdf>.

Pearson's observation was revisited by Fettis [12] half a century later, who rigorously established nonlinearity (numerically). In [9, Theorem 5.2], it is shown that for small $x > 0$,

$$p_5(0; x) = \sum_{k=0}^{\infty} r_{5,k} x^{2k+1}, \quad (29)$$

where

$$\begin{aligned} (15(2k+2)(2k+4))^2 r_{5,k+2} &= (259(2k+2)^4 + 104(2k+2)^2) r_{5,k+1} \\ &- (35(2k+1)^4 + 42(2k+1)^2 + 3) r_{5,k} + (2k)^4 r_{5,k-1}, \end{aligned} \quad (30)$$

with initial conditions $r_{5,-1} = 0$ and $r_{5,k} = \text{Res}_{s=-2k-2} W_5(0; s)$. Numerically, we thus find that

$$p_5(0; x) = 0.329934 x + 0.00661673 x^3 + 0.000262333 x^5 + O(x^7),$$

which reflects the approximate linearity of $p_5(0; x)$ for small x . Is this result beautiful because it entirely resolves the issue of whether the density is linear on $[0, 1]$ or is it ugly because it demolishes the apparent linearity?

The residue $r_{5,0} = p_5'(0; 0)$ can be shown to equal $p_4(0; 1)$. The so-called *modularity* of p_4 in the planar case [7], combined with the *Chowla–Selberg formula* [22], then permits us to obtain the amazing Gamma function closed-form

$$r_{5,0} = \frac{\sqrt{5}}{40} \frac{\Gamma(\frac{1}{15})\Gamma(\frac{2}{15})\Gamma(\frac{4}{15})\Gamma(\frac{8}{15})}{\pi^4}. \quad (31)$$

Moreover, high-precision numerical calculations lead to the conjectural evaluation [9, (5.3)]

$$r_{5,1} = \frac{13}{225} r_{5,0} - \frac{2}{5\pi^4} \frac{1}{r_{5,0}}, \quad (32)$$

and the recursion (30) implies that all coefficients $r_{5,k}$ in (29) can be expressed in terms of $r_{5,0}$. A dimensional recurrence then let us prove that this is true in all even dimensions since: *the originally conjectural relation (32) [9] is now proven* thanks to our work in dimension four [7].

Fancy that, we now can do inductions on both the number of steps and the dimension. Figure 4 and indeed the graphs in Figure 1 can be nicely rendered as animations. In doing so we view the dimensional parameter $\nu \geq 0$ as a real variable. While the dimension d was originally a whole number, we can now fruitfully think about $d = 2\nu + 2$ at values like π or $\sqrt{2}$. This may be dubious physics but it can lead to potent and beautiful mathematics, since J_ν is perfectly well defined for $\nu \geq 0, \nu \in R$.

7 Conclusion

Many more similar comments come to mind about other results in our suite of recent papers [6, 8, 9], but I content myself with one final remark.

Remark 7.1. (Meditation on beauty, III) We have shown that quite delicate results are possible for densities and moments of walks in arbitrary dimensions, especially for two, three and four steps. We find it interesting that induction between dimensions provided methods to show

equation (32), a result in the plane that we previously could not establish [9]. We also should emphasize the crucial role played by intensive computer experimentation and by computer algebra ('big data' meets modern computation). One stumbling block is that currently *Mathematica*, and to a lesser degree *Maple*, struggle with computing various of the Bessel integrals to more than a few digits — thus requiring considerable extra computational effort or ingenuity.

The seemingly necessary interplay from combinatorial to analytic to probabilistic tools and back, is ultimately one of the greatest sources of pleasure and beauty of the work. \diamond

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Jonathan M. Borwein, FRSC, FAA, FAMS
 CARMA, UNIVERSITY OF NEWCASTLE, AUSTRALIA
jonathan.borwein@newcastle.edu.au