Random Walk

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1 Introduction

In the following, some features of random walks were analysed. The first case examined was the 1-D random walk, which can be visualised as a walker moving on a wire. Next was the turn of the square 2-D lattice, followed by the triangular 2-D lattice and the circular random walk. In both dimensions and for all cases, the probability distributions that best fit the distributions of distances from the origin were then discussed. The self-avoiding random walk was then analysed: specifically, its algorithm was described and the value of the variance in relation to the number of steps was found analytically and numerically. Finally, an experimental proof of Polya's recurrence theorem through numerical simulations was provided.

2 1-D and 2-D Random Walk

2.1 1-D Lattice

A 1-D random walk can be thought as a point moving either on the left or on the right on a line. This walk can be visualised by plotting the position of the walker at each step on the line:

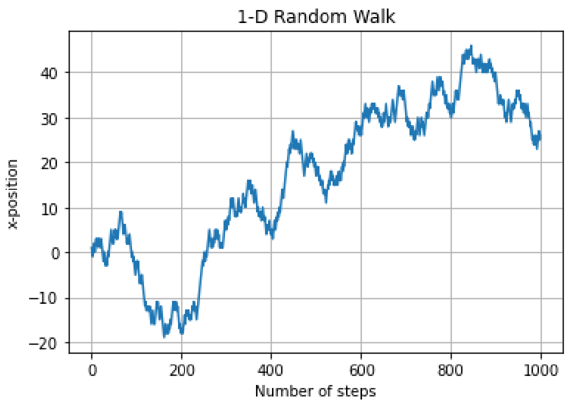

Figure 1: 1-D Random Walk with 1000 steps.

In 1-D, the two possible directions that the walker can take, have both probability equal to $\frac{1}{2}$.

The expectation value of each step is equal to zero:

$$\mathbb{E}[X_i] = \sum_{j=1}^{2} x_j p_j = (1)\frac{1}{2} + (-1)\frac{1}{2} = 0 \tag{1}$$

where $x_1 = 1$ and $x_2 = -1$.
Let S_0 be the starting point and S_N be the point where the walker will be after N steps. A random walk after N steps is defined as:

$$S_N = \sum_{i=1}^{N} X_i \tag{2}$$

and thus:

$$\mathbb{E}[S_N] = \mathbb{E}[\sum_{i=1}^{N} X_i] = \sum_{i=1}^{N} \mathbb{E}[X_i] = 0 \tag{3}$$

which means that after N steps the walker is expected to be at the starting point. Note that $E[S_N] = 0$ corresponds to the mean, μ. The variance is given by:

$$\sigma^2 = Var(S_N) = \mathbb{E}[(S_N - \mathbb{E}[S_N])^2] = \mathbb{E}[S_N^2] - \mathbb{E}[S_N] = N. \tag{4}$$

since:

$$\mathbb{E}[S_N^2] = \mathbb{E}[(\sum_{i=1}^{N} X_i)^2] = \mathbb{E}[\sum_{i=1}^{N} X_i^2 + \sum_{i \neq j} X_i X_j] \tag{5}$$

$$= \sum_{i=1}^{N} \mathbb{E}[X_i^2] + \sum_{i \neq j} \mathbb{E}[X_i X_j] = \sum_{i=1}^{N} 1 + \sum_{i \neq j} 0 = N \tag{6}$$

It turns out that evaluating a 1-D random walk n times for a fixed number of steps, N, the Probability Density Function (PDF) of the distances from the origin, $\{S_{N,1}, ..., S_{N,n}\}$, follows the PDF of the normal distribution with $\mu = 0$ and $\sigma = \sqrt{N}$.

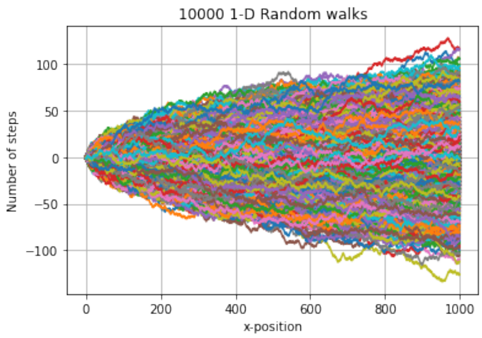

Figure 2: 10000 1-D Random walks, each with 1000 steps

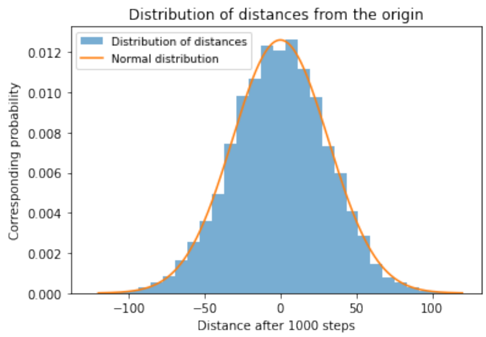

Figure 3: Distribution of distances and normal distribution, $scale = \sqrt{N}$

Furthermore, by calculating the distance between two points on the random walk that are a fixed number of steps, P, apart, it can be seen that these distances are non-randomly distributed. The distribution which best fits the values of the Euclidean distance of the random variables from the origin is the Chi distribution:

$$f(x,k) = \frac{x^{k-1}e^{-\frac{x^2}{2}}}{2^{\frac{k}{2}-1}\Gamma(k/2)} \quad for \;\; x \geq 0 \tag{7}$$

Where x is the Euclidean distance between two points P steps apart and k is the number of degree of freedoms. In the present case, $k = 1$ since the walker is moving on the x-line only:

$$f(x,1) = \sqrt{\frac{2}{\pi}}e^{-\frac{x^2}{2}} \tag{8}$$

Noting that, numerically, the variance of the distances was found to be linearly proportional to the step-distance and since the variance of (8) is 1, a scale parameter of $\frac{1}{\sqrt{P}}$ is needed for the data:

$$f(x) = \sqrt{\frac{2}{\pi P}}e^{-\frac{x^2}{2P}} \tag{9}$$

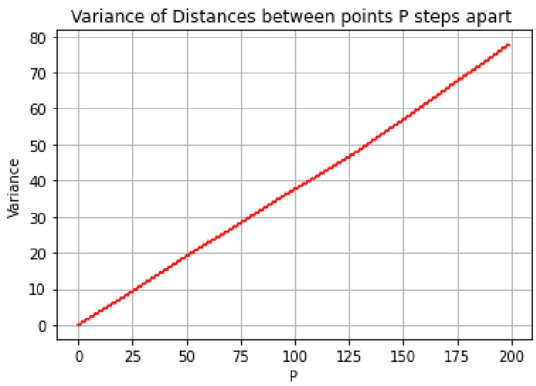

Figure 4: Variance of distances P steps apart, N = 100,000

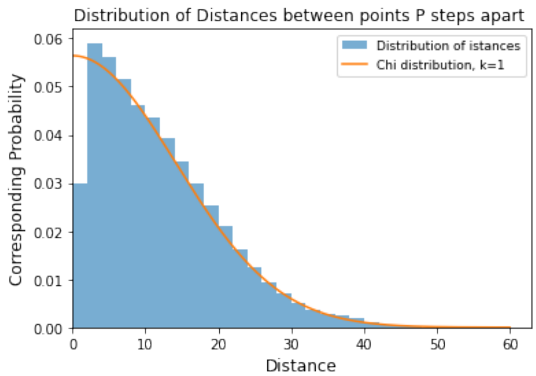

Figure 5: Distribution of distances and Chi distribution, $k = 1$ and $scale = \sqrt{N}$

A better visual proof of how well $f(x)$ fits the histogram of distances is given by the Cumulative Distribution Function (CDF) of $f(x)$ and the empirical Cumulative Distribution Function (eCDF) of the distances:

$$F(x) = \int_0^x f(t)\, dt = \int_0^x \sqrt{\frac{2}{\pi P}}e^{-\frac{t^2}{2P}}\, dt = erf(\frac{x}{\sqrt{2P}}) \tag{10}$$

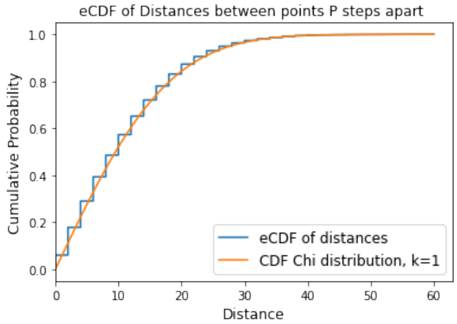

Figure 6: eCDF

2.2 2-D lattice

A 2-D random walk can be visualised by simply plotting its x and y positions:

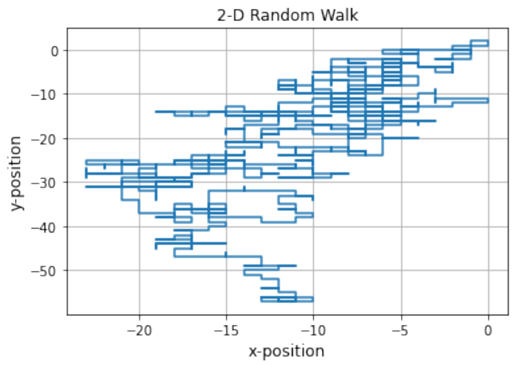

Figure 7: 2-D random walk with 1,000 steps

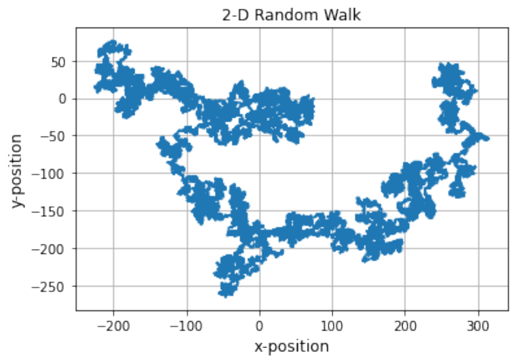

Figure 8: 2-D random walk with 100,000 steps

This walk is equivalent to two orthogonal 1-D random walks rotated by 45° and appropriately scaled.
Let Y_i and Z_i be the two independent random variables. If, at each step, the two walks are combined, the resulting walker will move in the following directions:

$$\mathbf{v_1} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \mathbf{v_2} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \quad \mathbf{v_3} = \begin{pmatrix} -1 \\ -1 \end{pmatrix}, \quad \mathbf{v_4} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{11}$$

Note: each vector has modulus $|\mathbf{v_j}| = \sqrt{2}$ and thus rotating the system by 45° degrees anticlockwise, the new vectors are:

$$\mathbf{v_1'} = \begin{pmatrix} 0 \\ \sqrt{2} \end{pmatrix}, \quad \mathbf{v_2'} = \begin{pmatrix} 0 \\ -\sqrt{2} \end{pmatrix}, \quad \mathbf{v_3'} = \begin{pmatrix} -\sqrt{2} \\ 0 \end{pmatrix}, \quad \mathbf{v_4'} = \begin{pmatrix} \sqrt{2} \\ 0 \end{pmatrix} \tag{12}$$

Finally, scaling the set $\{\mathbf{v_j}\}$ by multiplying it by $\frac{1}{\sqrt{2}}$, the final set of vectors $\{\mathbf{x_j}\}$ is obtained:

$$\mathbf{x_1} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \ \mathbf{x_2} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \ \mathbf{x_3} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \ \mathbf{x_4} = \begin{pmatrix} -1 \\ 0 \end{pmatrix} \tag{13}$$

which proves that a 2-D random walk is the combination of Y_i and Z_i both scaled by a factor of $\frac{1}{\sqrt{2}}$. As a consequence, the expectation value of the 2-D case for each step will be equal to zero:

$$\mathbb{E}[X_i] = \mathbb{E}[\frac{1}{\sqrt{2}}(Y_i + Z_i)] = \mathbb{E}[\frac{Y_i}{\sqrt{2}}] + \mathbb{E}[\frac{Z_i}{\sqrt{2}}] = \frac{1}{\sqrt{2}}(\mathbb{E}[Y_i] + \mathbb{E}[Z_i]) = 0 \tag{14}$$

$$\Rightarrow \mathbb{E}[S_N] = 0 \tag{15}$$

Consider:

$$R_N = \sum_{i=1}^{N} Y_i \quad and \quad T_N = \sum_{i=1}^{N} Z_i \tag{16}$$

Then:

$$Var(S_N) = Var(\frac{1}{\sqrt{2}}(R_N + T_N)) = (\frac{1}{\sqrt{2}})^2 \, Var(\frac{1}{\sqrt{2}}(R_N + T_N)) \tag{17}$$

$$= \frac{1}{2}[Var(R_N) + Var(T_N) + 2\, Cov(R_N, T_N)] \tag{18}$$

But from (4) and since the covariance of two independent variables is zero:

$$Var(S_N) = \frac{1}{2}[N + N] = N \tag{19}$$

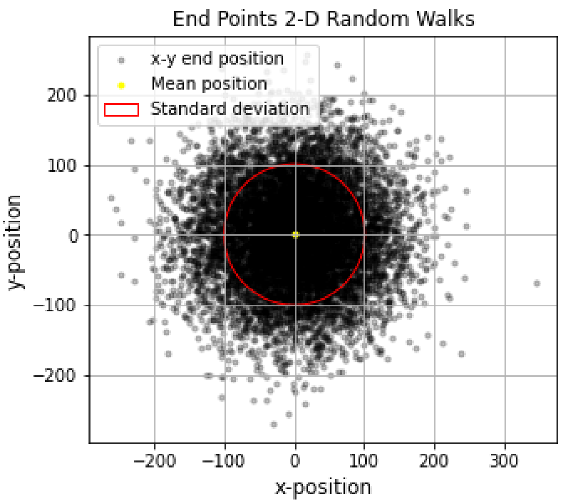

Figure 9: Scatter plot of the end points of 10,000 random walks with $N = 10,000$ each. The circle in red has radius equal to σ.

Also for this lattice, it is interesting to analyse the distribution of the Euclidean distances calculated at fixed step-distance. To fit this distribution, Chi with 2 degrees of freedom must be used. This corresponds to the Rayleigh distribution:

$$f(x,\sigma) = \frac{x}{\sigma^2} e^{-\frac{x^2}{2\sigma^2}} \tag{20}$$

and the corresponding CDF is given by:

$$F(x,\sigma) = 1 - e^{-\frac{x^2}{2\sigma^2}} \tag{21}$$

where σ is the so-called scale parameter. The first two moments can be found by using the Gaussian integral:

$$\int_0^\infty x^n e^{-ax^2} dx = \frac{\Gamma((n+1)/2)}{2a^{(n+1)/2}}, \quad a = \frac{1}{2\sigma^2} \tag{22}$$

The mean is given by (22) using $n = 2$:

$$\mu_1 = \int_0^\infty \frac{x^2}{\sigma^2} e^{-\frac{x^2}{2\sigma^2}} \, dx = \sigma\sqrt{\frac{\pi}{2}} \tag{23}$$

The second moment occurs when $n = 3$:

$$\mu_2 = \int_0^\infty \frac{x^3}{\sigma^2} e^{-\frac{x^2}{2\sigma^2}} \, dx = 2\sigma^2 \tag{24}$$

The variance is then:

$$Var(X) = \mu_2 - \mu_1^2 = \left(2 - \frac{\pi}{2}\right)\sigma^2 \tag{25}$$

where X is the random which has $f(x)$ as a PDF. In order to find σ, it is crucial to look at the relation between the variance and the step-length:

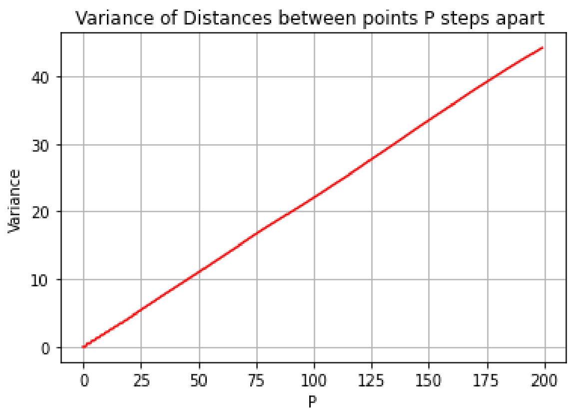

Figure 10: Variance of distances P steps apart, N = 100,000.

It stands out that the variance scales linearly with P and this implies that $\sigma^2 = C\frac{4-\pi}{2}P$ where C is a constant. To find C, we calculate the slop at every point of the graph and we take the average. The numerical value for the average slop is approximately 0.2207685532638581. Therefore:

$$C = 0.2207685532638581 \ \times \ \frac{4-\pi}{2} \approx 0.5143678096118238 \tag{26}$$

Please note this value is not fixed and it changes for every random walk. Repeating the simulation several times, it is possible to see that C oscillates between 0.20 and 0.23 and considering $N >> 1$, it is safe to pick $C = 0.20$ for the following simulations.
Implementing this into σ^2, one can observe how well Rayleigh's PDF and CDF fit the distances' distribution:

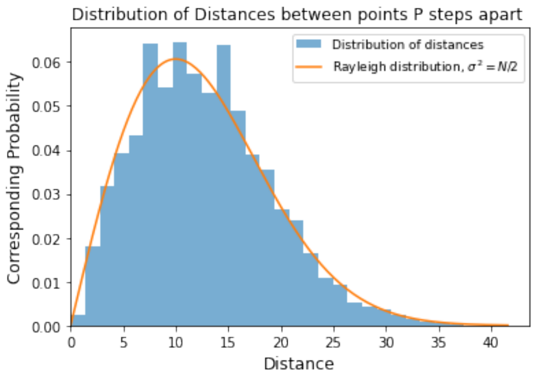

Figure 11: Distribution of distances and Rayleigh distribution, $N = 100,000$

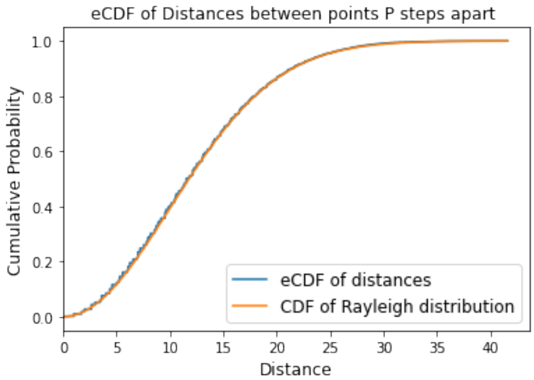

Figure 12: eCDF of distances and Rayleigh's CDF for a random walk of $N = 100,000$

2.3 Triangular 2-D random walk

Analogously to the square lattice example, the case of a 2-D random walk on a triangular lattice can also be decomposed into three 1-D random walks that are at an angle of 60° to each other.

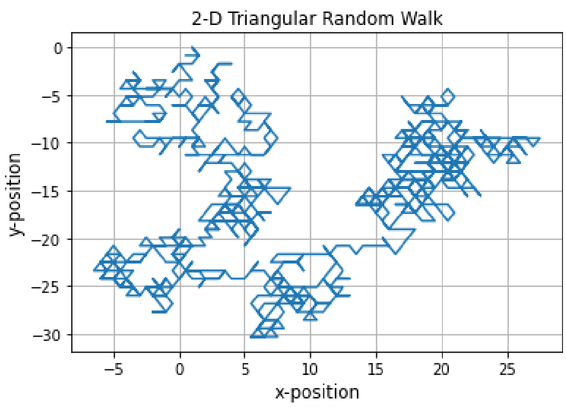

Figure 13: 2-D triangular random walk with 1000 steps.

The procedure is almost identical to that followed in the previous section and the directions which can be taken by the walker in this particular lattice are given by the following vectors:

$$\mathbf{x_1} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{x_2} = \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}, \quad \mathbf{x_3} = \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2}) \end{pmatrix}, \tag{27}$$

$$\mathbf{x_4} = \begin{pmatrix} -1 \\ 0 \end{pmatrix} \quad \mathbf{x_5} = \begin{pmatrix} -\frac{1}{2}) \\ -\frac{\sqrt{3}}{2} \end{pmatrix} \quad \mathbf{x_6} = \begin{pmatrix} \frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix} \tag{28}$$

Even though there are more directions of movement, the distribution of the distances between pair of points at a fixed number of steps apart still follows the probability density function of the Rayleigh distribution with the same scale parameter σ:

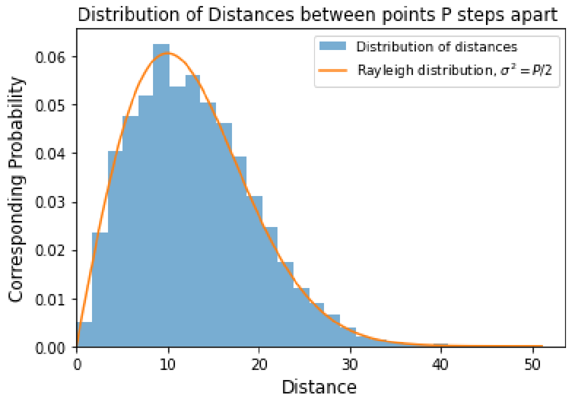

Figure 14: Distribution of distances using a triangular lattice, $N = 100,000$

Finally, one can clearly notice how the variance again scales linearly as N for N steps:

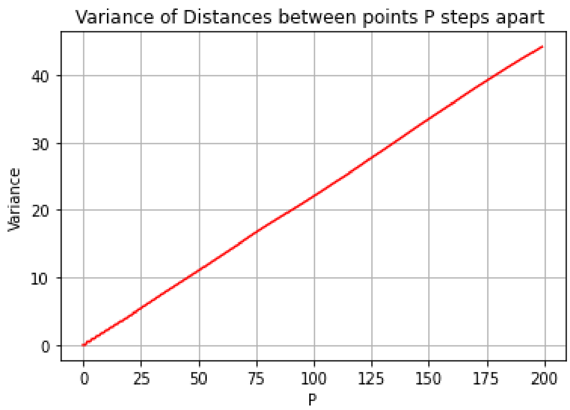

Figure 15: Variance of distances P steps apart using a triangular lattice, $N = 100,000$

2.4 Circular Random Walk

A particular case occurs when the 2-D walker is allowed to turn and travel at any angle, θ, between 0 and 2π after each step. The value of θ is random. The resulting random walk is the following:

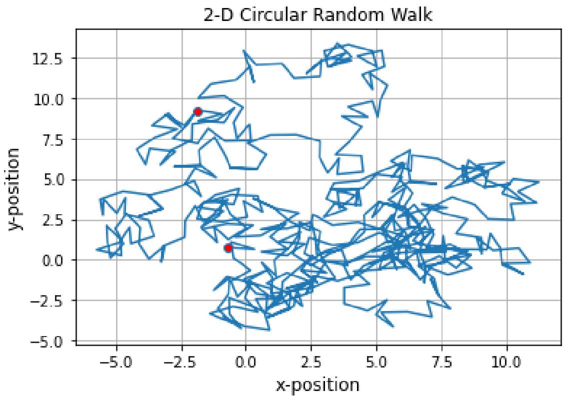

Figure 16: Circular random walk, $N = 500$

The possible directions are given by the set of vectors $\{\mathbf{x_j}\}$, where:

$$\mathbf{x_j} = \begin{pmatrix} \cos\theta_j \\ \sin\theta_j \end{pmatrix} \tag{29}$$

Running this type of walk n times with a fixed number N of steps per walk, and finding the Euclidean distance between the final point and the starting point, a new distribution of distances was found. The probability density function which fits this distribution was discovered by Kluyver[1] in 1905:

$$p(x; a_1, ..., a_N) = \int_0^\infty J_0(ux)J_0(ua_1)...J_0(ua_N)ux\,du \tag{30}$$

where $J_0(u)$ is the Bessel functions of the first kind of zeroth order:

$$J_0(u) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!\,\Gamma(m+1)} \left(\frac{u}{2}\right)^{2m} \tag{31}$$

and a_i are the lengths of each step, in the present case all equal to unity and thus:

$$p(x) = \int_0^\infty J_0(ux)[J_0(u)]^N ux\,du \tag{32}$$

Evaluating $p(x)$ numerically, resulted in the following curve:

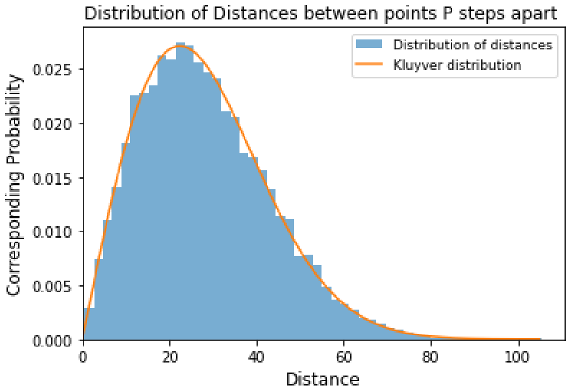

Figure 17: Distribution of distances for circular random walks with $N = 1,000$

Comparing $p(x)$ with Rayleigh distribution, it can be noticed that the first is wider and lower with a peak around 0.027 corresponding to a distance slightly above 20 while the latter is sharper and narrower.

3 Self-Avoiding Random Walk

A self-avoiding random walk (SAW) is a random walk which does not visit the same point more than once. The algorithm used to run this particular walk is not trivial and requires a longer computational time, so it is worth discussing how it works.

3.1 Algorithm

First of all, the initial position of the self-avoiding walker is set to be the origin and thus:

$$\mathbf{x_0} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow \mathbf{S_0} = [\mathbf{x_0}^T] \tag{33}$$

is the starting point. The four possible steps are given by (13). The SAW will be described by a matrix with 2 columns and N rows. In particular, the columns represent the x and y coordinates of the walker after every step and the step itself is indicated by the row on which the pair of coordinates are. The SAW can then be defined as:

$$\mathbf{S_N} = \begin{bmatrix} \mathbf{x_{0,j}} & \\ \mathbf{x_{1,j}} & \\ \mathbf{x_{2,j}} + \mathbf{x_{1,j}} & \\ . & . \\ . & . \\ . & . \\ \sum_{n=0}^{N} \mathbf{x_{n,j}} & \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ x_{1,j} & y_{1,j} \\ x_{2,j} + x_{1,j} & y_{2,j} + y_{1,j} \\ . & . \\ . & . \\ . & . \\ \sum_{n=0}^{N} x_{n,j} & \sum_{n=0}^{N} y_{n,j} \end{bmatrix} \tag{34}$$

where:

$$\mathbf{x_{n,j}} = \begin{pmatrix} x_j \\ y_j \end{pmatrix}, \quad j = 1, 2, 3, 4 \tag{35}$$

is one of the four possible vectors. The choice of j is random and equally probable.

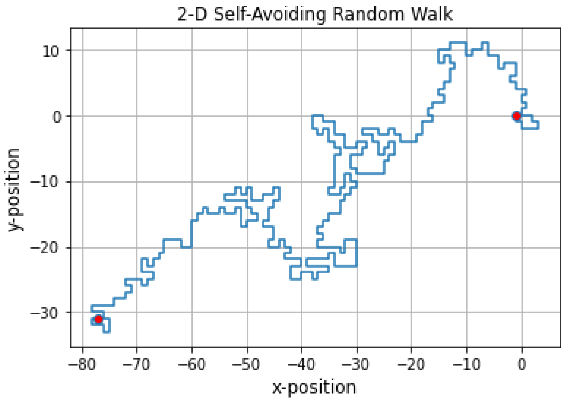

Figure 18: Self-avoiding random walk with $N = 1,000$

Assume N is the number of steps the walker is requested to take. In order to have a SAW, every time $\mathbf{S_n}$ is evaluated (for every $n \in (1, N]$), the n-th row of the matrix must not be equal to any of the other previous rows. In case this does not come true, the algorithm will remove the last row added to the matrix as well as $\mathbf{x_{n,j}}$ from the set of the four possible vectors. Then $\mathbf{S_n}$ is found by using one of the three remaining vectors and the SAW will carry on but not before resetting the set of possible vectors equal to the initial one i.e. $\{\mathbf{x_j}\} = \{\mathbf{x_1}, \mathbf{x_2}, \mathbf{x_3}, \mathbf{x_4}\}$. If there are no more vectors to choose from, the walk is interrupted and $\mathbf{S_n}$ is returned; otherwise, $\mathbf{S_N}$ is returned.
Note that a SAW could stop after only a few steps. For this reason, in order for the walker to reach a good distance, the algorithm was repeated using a $for\ loop$ until a Euclidean distance from the origin of 80 or more was obtained.

3.2 Variance

Until now, the variance has always been found to be linearly proportional to the number of steps. For the self-avoiding random walk the result is quite different but before showing it, it is worth mentioning an important aspect of the simulation used. In contrast to the computation of the variances for the previous cases, running a certain number of SAWs for a fixed step n would return some walks with n steps, but even more often walks with fewer steps than n. Therefore, to avoid discrepancies in the variances, simulations with n steps were carried on until a preset number of SAWs with actual n steps were found. Repeating this for $n \in [4, N]$, the below result was encountered.
The expected variance is still proportional with the number of steps, but in a non-linear way. In particular, the relation between the variance, σ^2, and the number of steps, N, is given by[2]:

$$\sigma^2 = DN^{2\nu} \tag{36}$$

Here ν is the so-called critical exponent which, in the 2-D case, was found to be equal to $\frac{3}{4}$. On the other hand, D is a constant which can be found numerically, minimising the sum of squared residuals with respect to D:

$$S = \sum_{n=1}^{N} (y_n - f(x_n))^2 = \sum_{i=1}^{N} (\sigma_n^2 - Dn^{3/2})^2 \tag{37}$$

Differentiating:

$$\frac{\partial S}{\partial D} = 0 = \sum_{n=1}^{N} (2Dn^3 - 2n^{\frac{3}{2}}\sigma_n^2) \tag{38}$$

Rearranging for D:

$$D = \frac{\sum_{n=1}^{N} n^{3/2}\sigma_n^2}{\sum_{n=1}^{N} n^3} \tag{39}$$

The value found for D is approximately 0.05747. Substituting this into (36) and plotting the equation for the variance against n, with $n \in [4, N]$, the following curve fitting is obtained:

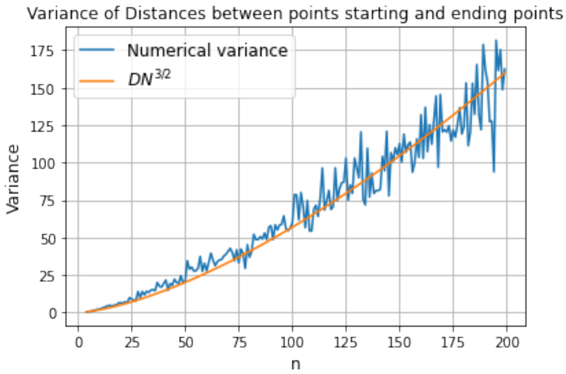

Figure 19: Fitted variance of distances from the origin; 200 samples per step

4 Polya's Recurrence Theorem

In this section, Polya's recurrence theorem is proved both theoretically and experimentally. The theorem states the following[3]: the simple random walk is *recurrent* in 1 and 2 dimensional lattices and it is *transient* for lattices with more than 2 dimension. A random walk is called *recurrent* if it returns to its starting position after a finite number of steps; otherwise, the walk is said to be *transient*.

4.1 Theoretical proof

Consider a 1-D walker and let S_n be the random walk he will take. Furthermore, let $P(S_n = 0)$ be the probability that the walker after n steps. It can be noticed that if n is odd, $P(S_n = 0) = 0$. It follows that:

$$\sum_{n=1}^{\infty} P(S_n = 0) = \sum_{n=1}^{\infty} P(S_{2n} = 0) \tag{40}$$

For 1-D, the walker must take an equal number number of steps to the right and to the left to get back to the origin. This implies that, for a walk of $2n$ steps, there are:

$$\binom{2n}{n} = \frac{(2n)!}{(n!)^2} \tag{41}$$

paths possible. Dividing (42) by the total number of possible paths i.e. 2^{2n}, $P(S_{2n} = 0)$ is found:

$$P(S_{2n} = 0) = \frac{(2n)!}{2^{2n}(n!)^2} \tag{42}$$

To simplify the latter, Stirling's formula is introduced:

$$n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n \tag{43}$$

Substituting:

$$P(S_{2n} = 0) \approx \frac{\sqrt{4\pi n}\left(\frac{2n}{e}\right)^{2n}}{2^{2n}\left(\sqrt{2\pi n}\left(\frac{n}{e}\right)^n\right)^2} = \frac{\sqrt{2}\,\sqrt{2\pi n}\,2^{2n}\left(\frac{n}{e}\right)^{2n}}{2^{2n}(2\pi n)\left(\frac{n}{e}\right)^{2n}} = \frac{1}{\sqrt{\pi n}} \tag{44}$$

The expected number of returns is:

$$\mathbb{E}[\sum_{n=1}^{\infty} \delta(S_{2n})] = \sum_{n=1}^{\infty} \mathbb{E}[\delta(S_{2n})] = \sum_{n=1}^{\infty} P(S_{2n} = 0) = \sum_{n=1}^{\infty} \frac{1}{\sqrt{\pi n}} \tag{45}$$

It is important to note that $\sum_{n=1}^{\infty} \frac{1}{n^p}$ diverges for $p \geq 1$ and converges for $p < 1$. This can be proved by applying the integral test for convergence:

$$\int_1^{\infty} \frac{1}{x^p} dx = \lim_{m \to +\infty} \int_1^m \frac{1}{x^p} dx = \lim_{m \to +\infty} \left(\frac{m^{1-p} - 1}{1 - p}\right) \tag{46}$$

This limit tends to a finite number, $\frac{1}{1-p}$, for $p > 1$ and to infinity for $p < 1$. In 1-D, $p = \frac{1}{2}$ which implies that the expected number of times the walker returns to the origin is infinity and therefore that the probability of returning to the origin equal to 1 as $n \to \infty$.
As showed previously, a 2-D random walk can be deconstructed into two 1-D walks and this implies that, for 2-D:

$$P(S_{2n} = 0) = \frac{1}{\sqrt{\pi n}} \times \frac{1}{\sqrt{\pi n}} = \frac{1}{\pi n} \tag{47}$$

which corresponds to the $p = 1$ case:

$$\int_1^{\infty} \frac{1}{x} dx = \Big[\log(x)\Big]_1^{\infty} \to \infty \tag{48}$$

Thus, also in the 2-D case the probability of returning to the origin is equal to 1.
The situation is different when the walker moves in 3-D. It can be shown[4] that in this respect:

$$P(S_{2n} = 0) = \frac{C}{n^{\frac{3}{2}}} \Rightarrow \sum_{n=1}^{\infty} P(S_{2n} = 0) < \infty \tag{49}$$

This implies that the probability of returning to the origin is less than 1 in 3-D i.e. the walker may not return to the starting point, no matter how many steps he will take. Glasser and Zucker[5] showed that $P(S_{2n} = 0) = 0.3405373296...$

4.2 Numerical proof

Going into the numerical part, the following results for the probabilities of the three walks were found:

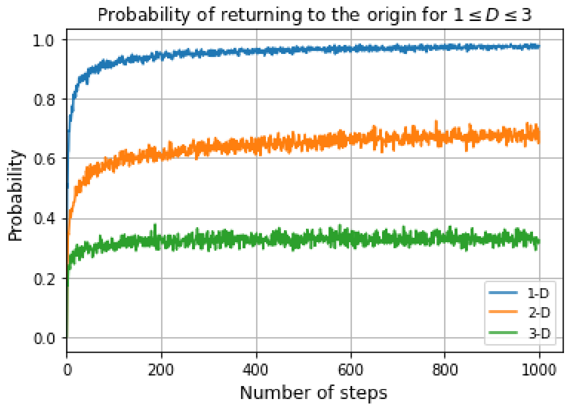

Figure 20: Probabilities of returning to the origin

One can observe that the 1 and 3-D plots coincide with the theoretical results. In particular, the mean value of the 3-D probabilities was found to be 0.322005, which differs with the theoretical value by about 0.018. It is less clear however that the 2-D graph tends to 1 as n becomes larger. Evaluating the expectation values, a similar scenario was found:

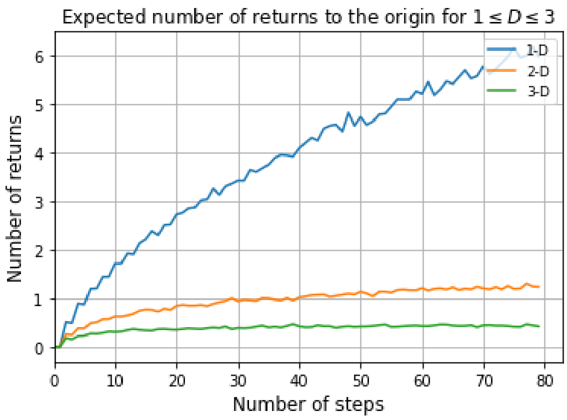

Figure 21: Expected number of returns to the origin

It stands out that the 3-D plot tends towards a number which was found to be 0.3823875; the 2-D plot goes to infinity as well as the 1-D one, although the latter goes much faster. The reason is that, as seen before, 2-D represents the limiting case of the p-series and follows $\log(n)$. Log does not have horizontal asymptotes and therefore tends to infinity as n goes to infinity but unfortunately it is not possible to prove this experimentally. Increasing the number of steps in simulations in order to improve this graph is also impractical given the relatively low computational power of the best modern computers.

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