Solutions to Problem Set 2b

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1 Non-reversing random walk

(a) Let $\Delta\vec{X}_n$ be the n-th step, with probability distribution

$$p(\Delta\vec{X}_n|\Delta\vec{X}_{n-1}) = -\frac{1}{2d-1}\delta(\Delta\vec{X}_n + \Delta\vec{X}_{n-1}) + \sum_{k=1}^{d}\frac{1}{2d-1}[\delta(\Delta\vec{X}_n - \vec{\sigma}_k) + \delta(\Delta\vec{X}_n + \vec{\sigma}_k)] \tag{1}$$

where $\vec{\sigma}_d$ is a vector on the direction of the d-th dimension, having the lattice spacing on that dimension as a modulus.

The probability that $\Delta\vec{X}_n = -\Delta\vec{X}_{n-1}$ (that is, a reversal) is zero by the above definition. The partial correlations can be seen directly from (1) to be

$$\langle\Delta\vec{X}_n^2\rangle_P = |\sigma_d|^2 \tag{2}$$

$$\langle\Delta\vec{X}_n\Delta\vec{X}_{n-1}\rangle_P = \rho|\sigma_d|^2 \tag{3}$$

$$\langle\Delta\vec{X}_n\Delta\vec{X}_{n-m}\rangle_P = 0, \quad \text{for } m \geq 2 \tag{4}$$

where the lattice spacings σ_d are supposed uniform for simplicity. The correlation ρ, assuming also $\sigma_d \cdot \sigma_{d'} = 0$ for $d \neq d'$ (i.e. orthogonal lattice axes), is

$$\rho = \frac{1}{2d-1} \tag{5}$$

The transition probability can be rewritten as

$$p(\Delta\vec{X}_n|\Delta\vec{X}_{n-1}) = -\rho\delta(\Delta\vec{X}_n + \Delta\vec{X}_{n-1}) + \bar{\rho}p(\Delta\tilde{X}) \tag{6}$$

where $p(\Delta\tilde{X})$ is the transition probability of a simple walk in the same lattice, and $\bar{\rho} = 1 + \rho$. But

$$p(\Delta\tilde{X}_{n-1}|\Delta\vec{X}_{n-2}) = -\rho\delta(\Delta\vec{X}_{n-1} + \Delta\vec{X}_{n-2}) + \bar{\rho}p(\Delta\tilde{X}) \tag{7}$$

therefore

$$p(\Delta\vec{X}_n|\Delta\vec{X}_{n-2}) = p(\Delta\vec{X}_n|\Delta\vec{X}_{n-1}) * p(\Delta\vec{X}_{n-1}|\Delta\vec{X}_{n-2}) = \bar{\rho}p(\Delta\tilde{X}) - \rho\bar{\rho}p(\Delta\tilde{X}) + \rho^2\delta(\Delta\vec{X}_n + \Delta\vec{X}_{n-2}) \quad (8)$$

and, analogously,

$$p(\Delta\vec{X}_n|\Delta\vec{X}_{n-3}) = \bar{\rho}p(\Delta\tilde{X}) - \rho\bar{\rho}p(\Delta\tilde{X}) + \rho^2\bar{\rho}p(\Delta\tilde{X}) - \rho^3\delta(\Delta\vec{X}_n + \Delta\vec{X}_{n-3}) \quad (9)$$

which can be simplified and generalized as

$$p(\Delta\vec{X}_m|\Delta\vec{X}_{m-m'}) = (1-(-\rho)^{m-m'})p(\Delta\tilde{X}) + (-\rho)^{m-m'}\delta(\Delta\vec{X}_m + \Delta\vec{X}_{m-m'}) \quad (10)$$

This result is used to obtain the correlation $c(m) = c(|m-m'|) = \langle\Delta\vec{X}_m\Delta\vec{X}_{m'}\rangle$. Since $\Delta\tilde{X}$ are not correlated by definition,

$$c(2) = \rho^2 \quad (11)$$
$$c(3) = \rho^3 \quad (12)$$
$$c(m) = \rho^m \quad (13)$$

The probability density for the total displacement $\vec{X}_n = \sum_{m=1}^{n}\Delta\vec{X}_m$ is $P(\vec{X}_n)$. This state may have been attained by a forward jump in the k-th dimension with probability $A_n^k(\vec{X})$, or by a backward jump in the same dimension, with probability $B_n^k(\vec{X})$. The probability is the sum of all these factors, properly scaled:

$$P_n(\vec{X}) = \rho\sum_{k=1}^{d} A_n^k(\vec{X}) + B_n^k(\vec{X}) \quad (14)$$

In the next step, the probabilities change to

$$A_{n+1}^k(\vec{X}) = \rho\sum_{l=1}^{d} A_n^l(\vec{X}-\vec{\sigma}_k) + \alpha_{kl}B_n^l(\vec{X}-\vec{\sigma}_k) \quad (15)$$
$$B_{n+1}^k(\vec{X}) = \rho\sum_{l=1}^{d} \alpha_{kl}A_n^l(\vec{X}-\vec{\sigma}_k) + B_n^l(\vec{X}-\vec{\sigma}_k) \quad (16)$$

where $\alpha_k l = 1$ if $k \neq l$, and 0 if $k = l$. This coefficient cancels the trajectories prohibited by the non-reversing condition. From the above evolution equations and the initial conditions

$$A_1^k(\vec{X}) = \frac{1}{2d}\delta(\vec{X}-\vec{\sigma}_k) \quad (17)$$
$$B_1^k(\vec{X}) = \frac{1}{2d}\delta(\vec{X}+\vec{\sigma}_k) \quad (18)$$

the evolution of the probabilities can be calculated.

In a continuum approximation, with $t = \tau n$, the probability $P_n(\vec{X})$ is $p(\vec{X}, t)$, as well as $A_n^k(\vec{X}) = a_n^k(\vec{X})$ and $B_n^k(\vec{X}) = b_n^k(\vec{X})$. In this notation,

$$p(\vec{X}, t) = \rho \sum_{k=1}^{d} a^k(\vec{X}, t) + b^k(\vec{X}, t) \tag{19}$$

and

$$a^k(\vec{X}, t+\tau) = \rho \sum_{l=1}^{d} a^l(\vec{X} - \vec{\sigma}_k, t) + \alpha_{kl} b^l(\vec{X} - \vec{\sigma}_k, t) \tag{20}$$

$$b^k(\vec{X}, t+\tau) = \rho \sum_{l=1}^{d} \alpha_{kl} a^l(\vec{X} + \vec{\sigma}_k, t) + b^l(\vec{X} + \vec{\sigma}_k, t) \tag{21}$$

Expanding (20) in Taylor series,

$$\begin{aligned} a^k + \tau a_t^k + \frac{\tau^2}{2} a_{tt}^k + \cdots = \\ \rho \sum_{l=1}^{d} a^l - \sigma_k a_{(k)}^l + \frac{\sigma_k^2}{2} a_{(kk)}^l + \cdots + \alpha_{kl} \left[b^l - \sigma_k b_{(k)}^l + \frac{\sigma_k^2}{2} b_{(kk)}^l + \cdots \right] \end{aligned} \tag{22}$$

where $a_t^k = \partial a/\partial t$, $a_{(k)}^l = \partial a / \partial x_k$ and $\sigma_k = |\vec{\sigma}_k|$. Analogously, for $b^k(\vec{X}, t)$,

$$\begin{aligned} b^k + \tau b_t^k + \frac{\tau^2}{2} b_{tt}^k + \cdots = \\ \rho \sum_{l=1}^{d} \left[\alpha_{kl} \left(a^l + \sigma_k a_{(k)}^l + \frac{\sigma_k^2}{2} a_{(kk)}^l + \cdots \right) + b^l + \sigma_k b_{(k)}^l + \frac{\sigma_k^2}{2} b_{(kk)}^l \cdots \right] \end{aligned} \tag{23}$$

Summing (22) and (23),

$$\begin{aligned} a^k + b^k + \tau(a_t^k + b_t^k) + \frac{\tau^2}{2}(a_{tt}^k + b_{tt}^k) + \cdots = \rho \left(p - \sigma_k q_{(k)} + \frac{\sigma_k^2}{2} p_{(kk)} + \cdots \right) + \\ \rho \sum_{l=1}^{d} \alpha_{kl} \left(a^l + b^l - \sigma_k (a_{(k)}^l - b_{(k)}^l) + \frac{\sigma_k^2}{2} (a_{(kk)}^l + b_{(kk)}^l) + \cdots \right) \end{aligned} \tag{24}$$

Summing (24) for $k = 1$ to d,

$$\begin{aligned} p + \tau p_t + \frac{\tau^2}{2} p_{tt} + \cdots = \rho \left(dp - \vec{\sigma} \cdot \nabla q + \frac{\sigma_d^2}{2} \nabla^2 p + \cdots \right) + \rho(d-1)p + \\ \rho \sum_{k=1}^{d} \sum_{l=1}^{d} \alpha_{kl} \left(-\sigma_k (a_{(k)}^l - b_{(k)}^l) + \frac{\sigma_k^2}{2} (a_{(kk)}^l + b_{(kk)}^l) + \cdots \right) \end{aligned} \tag{25}$$

d	$\langle n_{trap} \rangle$	$(\langle n_{trap}^2 \rangle - \langle n_{trap} \rangle^2)^{1/2}$
2	71.8	50.4
3	3676	3115

Table 1: Average and standard deviation of number of steps before trapping.

2 Self-trapping walk

The simulation of a self-trapping walk was performed recording the path of a walk in a list of positions optimized for quick access of spatially close points. A new move is selected randomly among all possible $2d$ directions. If the new position is blocked (or if the move is the reverse of the previous one), this particular move is ignored and a new move is chosen, until one free position is found, or all directions are found closed. If this happens, the walk is considered trapped.

An histogram of the number of steps before trapping $p(n_{trap})$ was constructed as shown in Figure 1. The average and standard deviation of n_{trap} are shown in Table 1 for $d = 2$ and $d = 3$. These simulations were performed with $n = 500$ and 100000 walks for 2-D and $n = 15000$ for 3-D. In four dimensions, trapping was an extremely low-probability event even for $n = 1000000$ and appeared to be uniformly distributed over the values of n from the few (1000) samples.

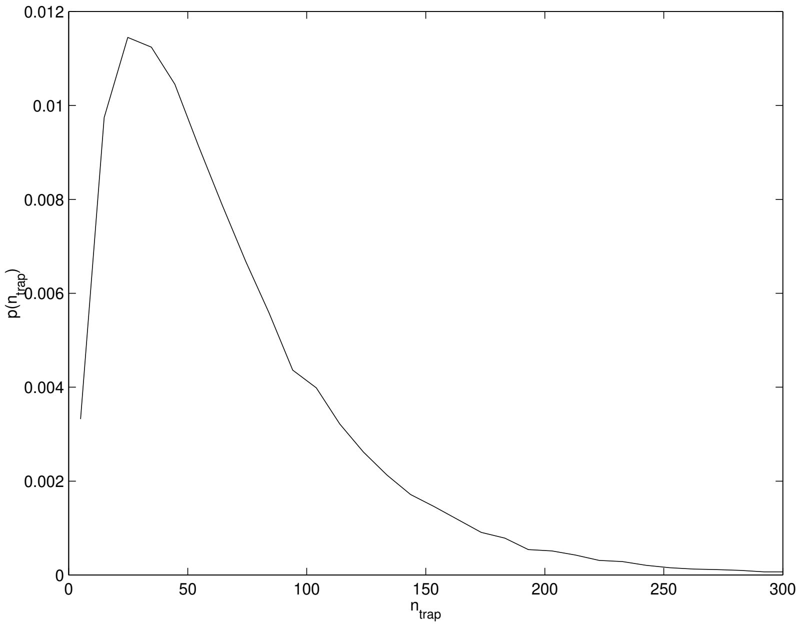
The position distribution after n steps was also obtained for certain values of n, as shown in Figures 2 and 3. For 2-D, since most walks are trapped around $n = 70$ steps, the distribution quickly converges to a stationary value. For 3-D, the distribution slowly widens while keeping the peak position, until convergence at a larger n. Finally, in the 4-D case the distribution behaves similarly to a random walk, and shows no sign of convergence.

3 Self-avoiding walk

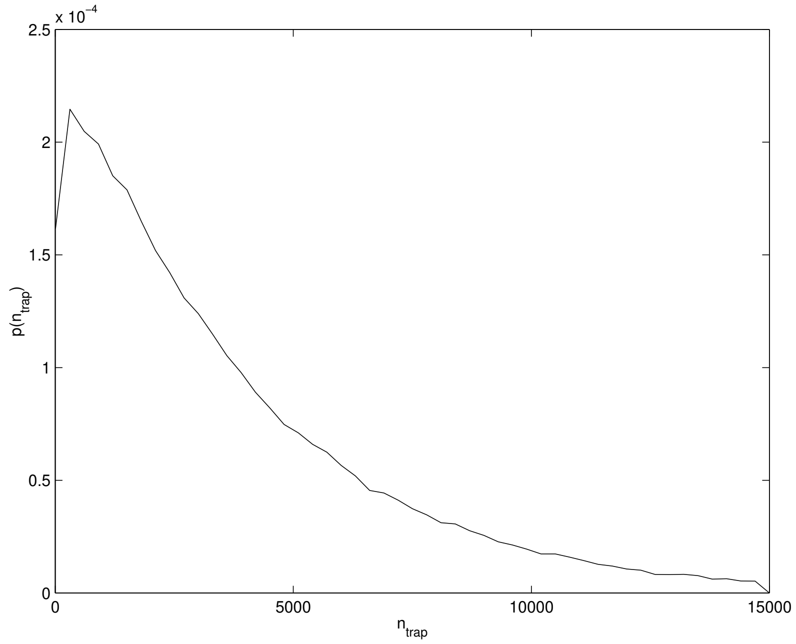
This kind of walk was simulated using the principles described in the previous section, except the treatment of the trapping. When a walker is trapped, it steps back until there is any unvisited position to move to, and continues, avoiding all visited positions including those which it has just stepped back from. This approach was apparently successful and large values of n were made possible, as shown for example in Figure 4.

For 2-D, 100000 walks of length 2000 were performed. For 3-D and 4-D, 10000 walks of length 20000 were used. The probability distributions for the position after n steps are shown in Figure 5, for $d = 2, 3$ and 4. The root-mean-square length was also plotted in a log-log scale in Figure 7, and from these the scaling coefficients in Table 2 were determined. As expected, the scaling for 4-D is the same as that of a random walk.

It seems that the method constructs biased walks, because the scaling exponents were not obtained as expected. Repeating the walks for smaller values of n did not help. For 2-D and $n_{max} = 200$, a scaling exponent $\nu \approx 0.5764$ was obtained, hardly an improvement over the previous value. The correctness of the implementation (not the algorithm, which is obviously flawed) was checked by running the 1-D case, where the exponent $\nu = 1$ was obtained.

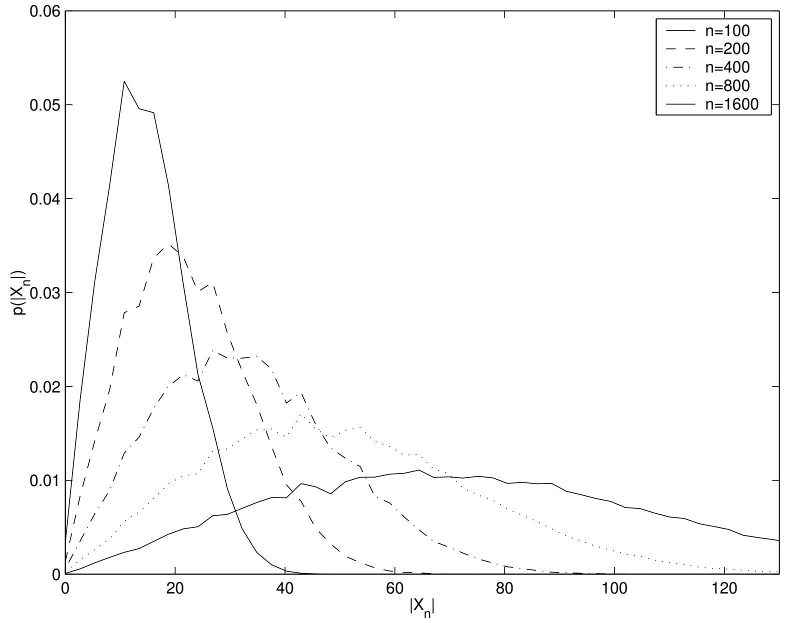


(a) $d = 2$

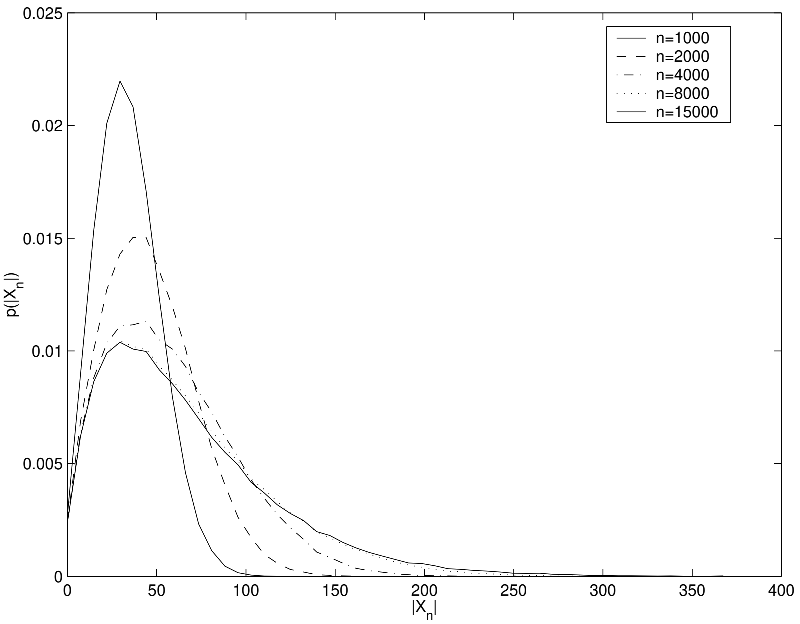


(b) $d = 3$

Figure 1: Probability density for the number of steps before trapping $p(n_{trap})$.

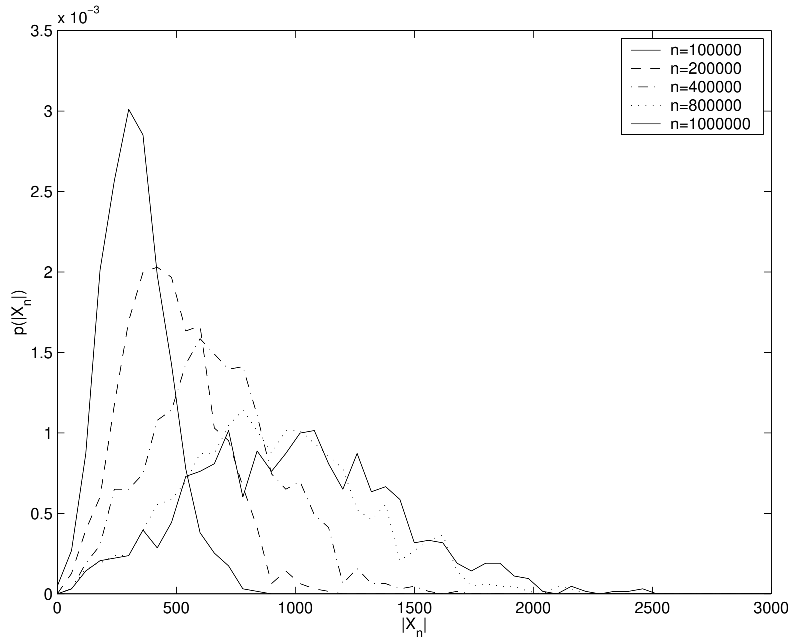


(a) $d = 2$



(b) $d = 3$

Figure 2: Probability density for the position $p(|X_n|)$ of a self-trapping walk.



(a) $d = 4$

Figure 3: Probability density for the position $p(|X_n|)$ of a self-trapping walk.

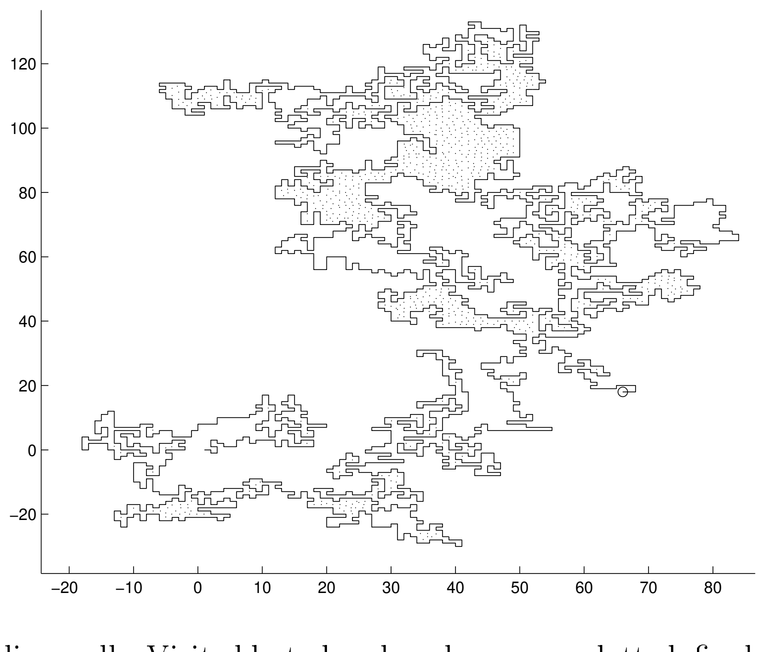
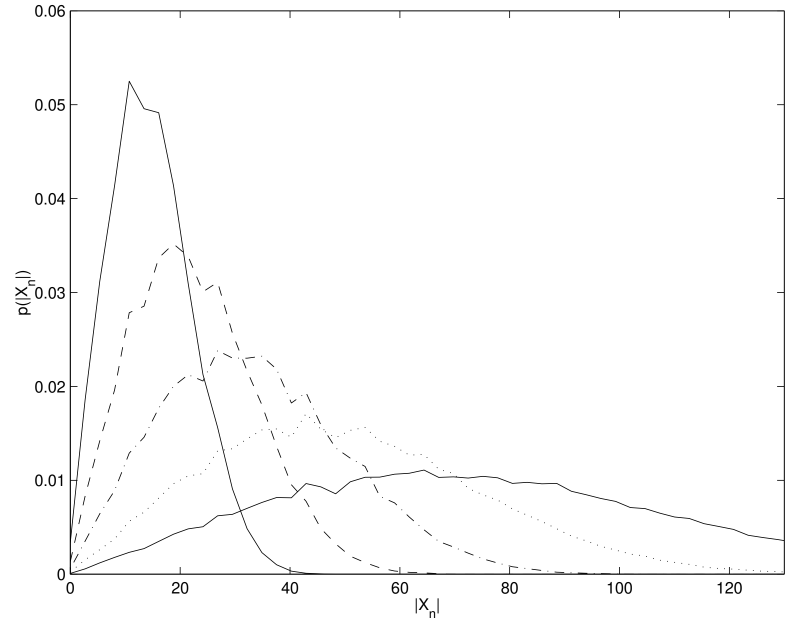
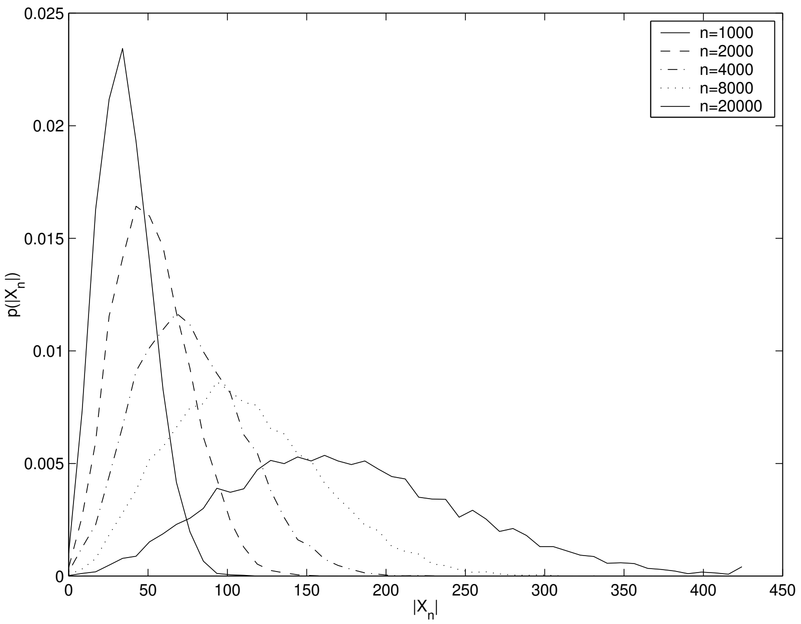


Figure 4: Self-avoiding walk. Visited but abandoned areas are dotted, final path is continuous. The walker started at the origin and is at the circle after $n = 3300$ steps.



(a) $d = 2$

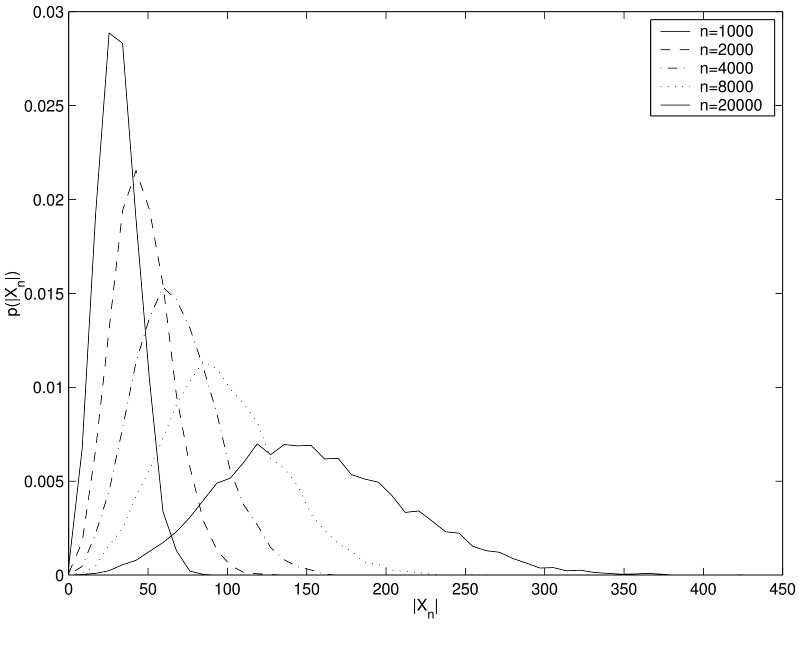


(b) $d = 3$

Figure 5: Probability density for the position $p(|X_n|)$ of a self-avoiding walk.

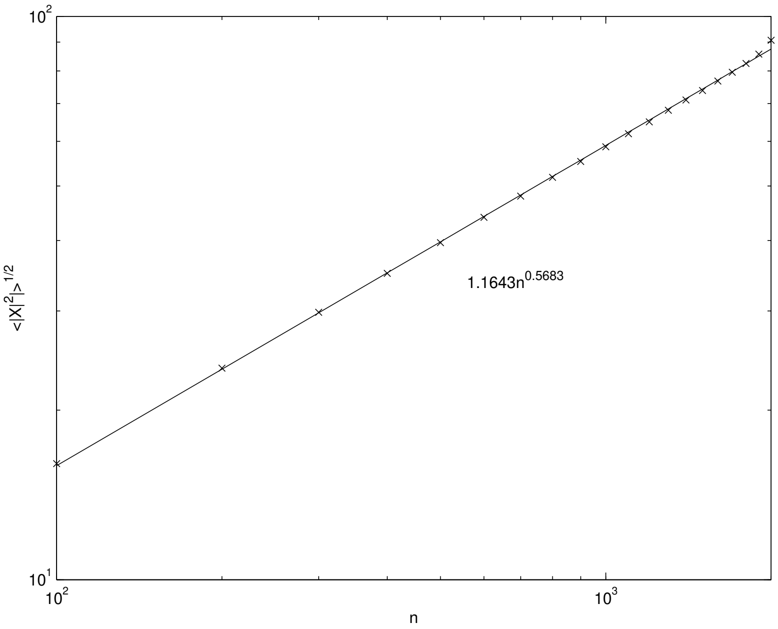
d	ν	expected
2	0.5683	0.75
3	0.5058	≈ 0.5877
4	0.4995	≈ 0.5

Table 2: Scaling coefficients.

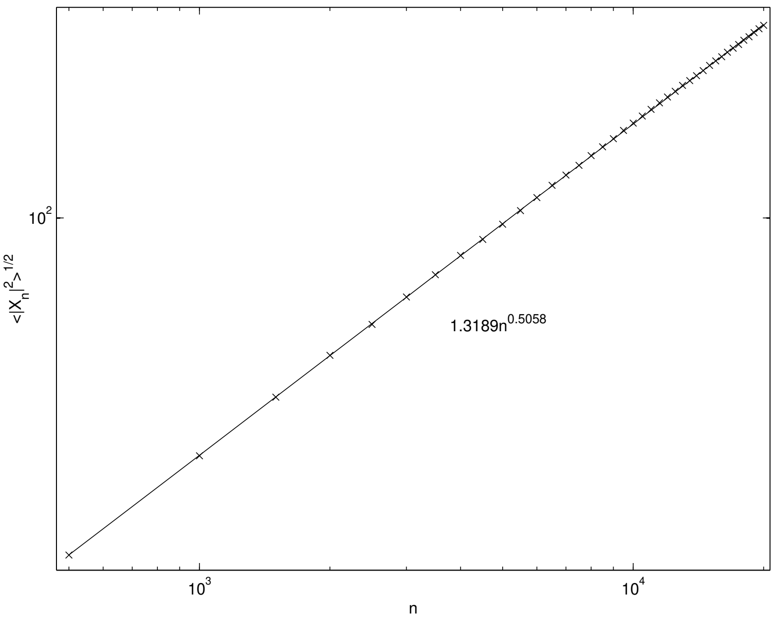


(a) $d = 4$

Figure 6: Probability density for the position $p(|X_n|)$ of a self-avoiding walk.

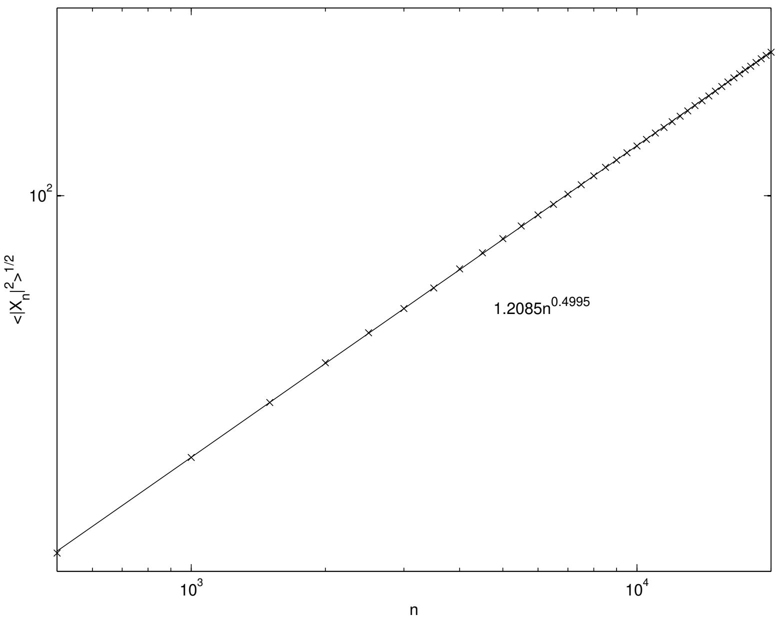


(a) $d = 2$



(b) $d = 3$

Figure 7: Average root-mean-square position after n steps.



(a) $d = 4$

Figure 8: Average root-mean-square position after n steps.