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On the Large Deviations Rate Function for Symmetric Simple Random Walk in Dimension $d \in \mathbb{Z}_+$

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Abstract. The large deviations rate function $\Lambda^{(d)}$ of d-dimensional symmetric simple random walk $S^{(d)}(n)$ describes the log-asymptotic behavior of the fundamental probability $P(S^{(d)}(n) = x)$ in the large deviations regime, that is, when $n = \mathcal{O}(\|x\|)$, but also in the so-called moderate deviations regime, that is, when $n^{1/2} = o(\|x\|)$ and $\|x\| = o(n)$. In Beneš (2019), we provided precise asymptotics for $P(S^{(d)}(n) = x)$ in dimensions 1 and 2 and, as an immediate consequence, we obtained $\Lambda^{(d)}$ for $d = 1$ and $d = 2$. The techniques developed in that paper do not translate readily to higher dimensions. In the present paper, we show that for $d \in \mathbb{Z}_+$,

$$\Lambda^{(d)}(\alpha) = \log d + \frac{1}{2}\sum_{i=1}^{d}\big((a_i+\alpha_i)\log(a_i+\alpha_i) + (a_i-\alpha_i)\log(a_i-\alpha_i)\big),$$

where $\alpha = (\alpha_1, \ldots, \alpha_d)$ satisfies $\sum_{i=1}^d |\alpha_i| \leq 1$. The quantities $a_i = a_i(\alpha)$ are not explicit but are given in terms of the solution of a system of quadratic equations. This result represents partial progress towards the generalization of the results in Beneš (2019) to any dimension $d \in \mathbb{Z}_+$.

1. Introduction

Consider a symmetric simple random walk $S^{(d)}$ in dimension $d \in \mathbb{Z}_+$, defined by $S^{(d)}(0) = 0$ and for $n \in \mathbb{Z}_+$, by $S_n^{(d)} = \sum_{k=1}^n X_k^{(d)}$, where $\{X_k^{(d)}\}_{k\in\mathbb{Z}_+}$ are independent random vectors satisfying $P(X_k^{(d)} = \pm e_i) = \frac{1}{2d}, i = 1, \ldots, d$, and $\{e_i\}_{i\in\{1,\ldots,d\}}$ is the standard orthonormal basis of $\mathbb{R}^d$.

The study of the probability

$$P(S_n^{(d)} = x), \tag{1.1}$$

that d-dimensional symmetric simple random walk $S^{(d)}$ started at the origin is at a given location $x = (x_1, \ldots, x_d) \in \mathbb{Z}^d$ at time $n \in \mathbb{Z}_+$ has a long history, dating back to over a century ago (see Pólya (1921)). Khintchine (1929) provided a close to complete solution to the problem in dimension 1, and since then, the analysis of the probability in (1.1), both for simple random walk and more

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general walks has continued to be developed in an important body of work, from Cramér (1938) to more recent results of varying levels of generality (see for instance Borovkov and Mogulskii (1999), Lawler (1991), Lawler and Limic (2010), or Beneš (2019)), some of which rely on the fundamental developments of large deviations theory in Varadhan (1966). See the Appendix in Beneš (2019) for a brief historical description of the evolution of this area of probability theory.

Let (here and throughout this paper) $\|\cdot\|_p$ denote the L^p norm. If $\sum_{i=1}^d x_i + n$ is even, the probability in (1.1) is, as suggested by the multidimensional central limit theorem, asymptotic to

$$2(d/2\pi n)^{d/2} \exp\{-d\|x\|_2^2/2n\} \tag{1.2}$$

when $\|x\|_2$ is of order up to $\sqrt{n}$ (see Lawler (1991), Section 1.2). It turns out that the same is true when $\|x\|_2$ is of order less than $n^{3/4}$ (see Lawler and Limic (2010), Section 2.3.1). However, this is as far as the expression in (1.2) is valid. Indeed, we showed in Beneš (2019) that in the two-dimensional case, the quantity (1.2) ceases to describe the probability in (1.1) when $\|x\|_2$ is of order greater than $n^{3/4}$. For such x, there are correction terms in the exponent of (1.2) which cause the probability to decay faster, which is unsurprising, since for $\|x\|_1 > n, P(S^{(d)}(n) = x) = 0$. The number of such correction terms grows with $\|x\|_2$ and tends to infinity as $\|x\|_1 \to n$. See Theorem 2.2 and Figure 1 in Beneš (2019) for more details. One interesting consequence of the expression obtained in Beneš (2019) for the probability in (1.1) is that the position at time n of planar simple random walk is approximately (in a sense that is made precise in that paper) rotationally symmetric if one considers points in any disk of radius $o(n^{3/4})$ but is not approximately rotationally symmetric for points outside of any disk of radius of order greater than $n^{3/4}$.

The questions discussed above can be viewed through the lens of large deviations theory. Indeed, it is known (see the Appendix in Beneš (2019) for a brief discussion of the historical development of the general theory encompassing this statement) that there exists a function $\Lambda = \Lambda^{(d)}$ such that, as $n \to \infty$,

$$\log P(S_n^{(d)} = x) \sim -n\Lambda(\alpha), \tag{1.3}$$

where $\alpha = x/n$. Λ is called the large-deviations rate function, also known as the Legendre-Fenchel transform of the logarithm of the moment-generating function M, defined as follows:

$$\Lambda(\alpha) = \sup_{\lambda \in \mathbb{R}^d} \{\langle \lambda, \alpha \rangle - \log M(\lambda)\},\ \alpha \in \mathcal{X} \tag{1.4}$$

Here $\mathcal{X} = \{x \in \mathbb{R}^d : \|x\|_1 \leq 1\}$ is the convex hull of the points of the increment distribution of symmetric simple random walk in $\mathbb{Z}^d$.

In dimension 1, it is easy to verify that

$$\Lambda(\alpha) = \frac{1}{2}\big((1+\alpha)\log(1+\alpha) + (1-\alpha)\log(1-\alpha)\big) \tag{1.5}$$

satisfies equation (1.4). Note that this is also a consequence of Theorem 2.1 in Beneš (2019).

In dimension 2, it takes substantially more work (see Beneš (2019)) to verify that with $\alpha = (\alpha_1, \alpha_2)$,

$$\begin{aligned} \Lambda(\alpha) \quad = \quad & \frac{1}{2}\Big((1+\alpha_1+\alpha_2)\log(1+\alpha_1+\alpha_2) + (1+\alpha_1-\alpha_2)\log(1+\alpha_1-\alpha_2) \\ & +(1-\alpha_1+\alpha_2)\log(1-\alpha_1+\alpha_2) + (1-\alpha_1-\alpha_2)\log(1-\alpha_1-\alpha_2)\Big) \end{aligned} \tag{1.6}$$

satisfies equation (1.4). In dimension d, solving equation (1.4) for simple random walk would require finding, for $\alpha \in \mathcal{X}$, the supremum over all $\lambda = (\lambda_1, \ldots, \lambda_d) \in \mathbb{R}^d$, of

$$\Lambda(\alpha) = \sum_{i=1}^d \lambda_i \alpha_i - \log\left(\frac{1}{d}\sum_{i=1}^d \cosh(\lambda_i)\right),$$

which would be achieved by solving for λ the system of equations

$$\alpha_j = \frac{\sinh(\lambda_j)}{\sum_{i=1}^d \cosh(\lambda_i)}, \quad j \in \{1, \ldots, d\}.$$

This is beyond our technical ability in dimension 3 and rapidly becomes more difficult as the dimension increases.

Another approach to seeking a solution to (1.4) would be to look for natural higher-dimensional extensions of the expressions in (1.5) and (1.6) and verify that they indeed provide the supremum in (1.4). One might guess, for instance, that

$$\Lambda(\alpha) = \sum_{x \in \mathcal{C}} (1 + \langle x, \alpha \rangle) \log(1 + \langle x, \alpha \rangle),$$

where $\alpha \in \mathbb{R}^d$ and $\mathcal{C}$ is the set consisting of the 2^d points in $\mathbb{R}^d$ for which each coordinate is either -1 or 1. However, a straightforward but algebraically tedious calculation shows that this function is not a solution to (1.4) when $d = 3$. Other natural guesses had to be similarly excluded after direct calculation showed they didn't solve (1.4).

The approach we take in this paper is probabilistic (as opposed to an analytic approach focused on solving (1.4) directly): If one considers a d-dimensional simple random walk's steps only at the times it moves along a specific dimension, those steps constitute a one-dimensional simple random walk along that dimension. This fact, together with Theorem 2.1 in Beneš (2019), can be used to express the probability in (1.1) as follows: If for $1 \le i \le d, N_i = N_i(n)$ is the number of steps the random walk takes along the ith dimension, then it follows from conditional independence of the behavior of the walk in each of the d dimensions that for $\|x\|_1 \le n$ such that $\|x\|_1 + n$ is even,

$$\begin{aligned} P(S^{(d)}(n) = x) &= \sum P(N_1 = n_1, \ldots, N_d = n_d) \prod_{i=1}^d P(S^{(1)}(n_i) = x_i) \\ &\sim \frac{1}{d^n} \sum \binom{n}{n_1, \ldots, n_d} \prod_{i=1}^d \sqrt{\frac{2}{\pi n_i}} \frac{1}{\sqrt{1 - (n_i/n)^2}} \exp\left(- \sum_{\ell=1}^{\infty} \frac{1}{2\ell(2\ell - 1)} \frac{x_i^{2\ell}}{n_i^{2\ell - 1}} \right), \end{aligned} \tag{1.7}$$

where the sum is over all vectors $(n_1, \ldots, n_d)$ such that $\sum_{i=1}^d n_i = n$ and subject to the requirement that $n_i \ge |x_i|$ for all $1 \le i \le d$.

This expression is not particularly useful for any practical purposes and obtaining a convenient expression in terms of elementary functions of x and n, valid in both the moderate and large deviation regimes, is far from trivial outside of the one-dimensional case. In dimension one, this expression was found in Khintchine (1929) and slightly refined in Beneš (2019); the two-dimensional case is resolved in Beneš (2019), using the idea that a two-dimensional simple random walk can be thought of in terms two independent one-dimensional random walks on diagonal lattices (see Beneš (2019) for details). This idea unfortunately cannot be used in higher dimensions, which implies that finding asymptotics for (1.1) is likely difficult in the large deviations regime in dimension 3 and higher. However, the log-asymptotic behavior is given by Λ, for which we derive an expression in terms of elementary functions that depend on the solutions of systems of quadratic equations which we did not manage to solve.

2. Statement of Result

The theorem below gives an expression for the simple random walk large deviations rate function in all integer dimensions. The expression is not explicit, but can be made so if one manages to solve equations (2.2) and (2.3) below.

Theorem 2.1. *Suppose $S^{(d)}$ is d-dimensional simple random walk. Then for $x \in \mathbb{Z}^d$ with $\sum_{i=1}^d x_i + n$ even and such that $\|x\|_1 \leq n$, we have*

$$\log P(S^{(d)}(n) = x) \sim -n\Lambda(\alpha),$$

with

$$\Lambda(\alpha) = \log d + \frac{1}{2}\sum_{i=1}^{d}\left((a_i + \alpha_i)\log(a_i + \alpha_i) + (a_i - \alpha_i)\log(a_i - \alpha_i)\right), \tag{2.1}$$

where $\alpha = (\alpha_1, \ldots, \alpha_d) = x/n$ and the parameters $a_i \geq 0, i = 1, \ldots, d$, satisfy

$$\sum_{i=1}^{d} a_i = 1 \tag{2.2}$$

and for $1 \leq j \leq d-1$,

$$a_j^2 - \alpha_j^2 = a_d^2 - \alpha_d^2. \tag{2.3}$$

Note 2.1. In the case where $d = 2$, this theorem says that

$$\begin{aligned}\Lambda(\alpha) \quad = \quad & \log 2 + \frac{1}{2}\big((\alpha_1 + a_1)\log(\alpha_1 + a_1) + (\alpha_1 - a_1)\log(\alpha_1 - a_1) \\ & +(\alpha_2 + 1 - a_1)\log(\alpha_2 + 1 - a_1) + (\alpha_1 - (1 - a_1))\log(\alpha_1 - (1 - a_1))\big)\end{aligned} \tag{2.4}$$

with

$$a_1 = \sqrt{a_2^2 - (\alpha_2^2 - \alpha_1^2)}.$$

and $a_1 + a_2 = 1$. These two equations imply

$$\sqrt{a_2^2 - (\alpha_2^2 - \alpha_1^2)} + a_2 = 1,$$

which is the case if and only if

$$a_2^2 - (\alpha_2^2 - \alpha_1^2) = 1 - 2a_2 + a_2^2 \iff a_2 = \frac{1 + \alpha_2^2 - \alpha_1^2}{2} \iff a_1 = \frac{1 + \alpha_1^2 - \alpha_2^2}{2}.$$

Plugging these values into (2.4) yields, as expected, (1.6).

Note 2.2. If one solves equations (2.2) and (2.3), the solution will readily yield an explicit large deviations rate function for d-dimensional symmetric simple random walk. In dimension 3, solving this set of equations amounts to solving the following quartic equation for α_3:

$$a_3^4 - \frac{4}{3}a_3^3 + \frac{2}{3}(\alpha_1^2 + \alpha_2^2 - 2\alpha_3^2 - 1)a_3^2 - \frac{4}{3}(\alpha_1^2 + \alpha_2^2 - 2\alpha_3^2 - 1)a_3 + \frac{1}{3}(2\alpha_1^2 + 2\alpha_2^2 - 4\alpha_3^2 - \alpha_1^4 - \alpha_2^4 + 2\alpha_1^2\alpha_2^2 - 1) = 0.$$

While this is in principle solvable, it is computationally arduous and the output we obtained from computer algebra systems was exceedingly complicated to be useful for any practical purposes.

Note 2.3. While solving equations (2.2) and (2.3) is challenging, even in dimension 3, it is relatively easy to solve in the case $a_1 = a_2 \neq a_3$. Indeed, in that case, one can show that

$$\begin{aligned} a_1 &= \frac{1}{3}\left(2 - \sqrt{1 - 3\left(\left(\frac{\alpha_1 + \alpha_2}{2}\right)^2 - \alpha_3^2\right)}\right) = a_2, \\ a_3 &= \frac{1}{3}\left(2\sqrt{1 - 3\left(\left(\frac{\alpha_1 + \alpha_2}{2}\right)^2 - \alpha_3^2\right)} - 1\right). \end{aligned}$$

This doesn't readily yield the general solution (a_1, a_2, a_3) as a function of $(\alpha_1, \alpha_2, \alpha_3)$, but we hope it might be used together with the fact that the solution must satisfy some symmetry properties to provide candidates for a solution to equations (2.2) and (2.3). All our attempts in this direction were unfortunately unsuccessful.

3. Proof of Theorem 2.1

Consider $\alpha = (\alpha_1, \ldots, \alpha_d)$ with $\|\alpha\|_1 \le 1$ such that $n\alpha \in \mathbb{Z}^d$ and $n + n\sum_{i=1}^d \alpha_i$ is even. Let $N = (N_1, \ldots, N_d)$, where

$$N_i = \sum_{j=1}^{n} I\{\langle S_j - S_{j-1}, e_i\rangle \neq 0\},$$

where $\langle \cdot, \cdot \rangle$ denotes the scalar product in $\mathbb{R}^d$ and I is the indicator function. Clearly, since the number of terms in the sum in (1.7) is polynomial in n, using the notation $f(n) \approx g(n)$ to mean that $\log f(n) \sim \log g(n)$, we have, with $a = (a_1, \ldots, a_d) \in \mathbb{R}^d$ such that $\|a\|_1 = 1$,

$$P(S^{(d)}(n) = n\alpha) \approx \sup_a P\left(S^{(d)}(n) = n\alpha, N = na\right).$$

Without loss of generality, we use that fact that the probability above is an even function in each of its coordinates, to assume from here on that $a_i \ge 0$ for all i in the supremum above. In particular, this assumption implies that

$$\sum_{i=1}^{d} a_i = 1.$$

Note that by conditional independence of the walks' steps along each dimension,

$$\begin{aligned} P(S^{(d)}(n) = n\alpha, N = na) &= P(N = na)\prod_{i=1}^{d} P(S^{(1)}(na_i) = n\alpha_i) \\ &= \left(\frac{1}{d}\right)^n \binom{n}{na_1, \ldots, na_d} \prod_{i=1}^{d} P(S^{(1)}(na_i) = n\alpha_i). \qquad (3.1) \end{aligned}$$

Combining (1.3) and (1.5) implies that this last term equals

$$\left(\frac{1}{d}\right)^n \binom{n}{na_1, \ldots, na_d} \prod_{i=1}^{d} \exp\Big(-\frac{na_i}{2}\left((1+\alpha_i/a_i)\log(1+\alpha_i/a_i) + (1-\alpha_i/a_i)\log(1-\alpha_i/a_i)\right)\Big). \qquad (3.2)$$

Note that Stirling's formula and the fact that $\sum_{i=1}^d a_i = 1$ imply that

$$\begin{aligned} \log\binom{n}{na_1, \ldots, na_d} &= \log\frac{n!}{\prod_{i=1}^d (na_i)!} \sim \log\frac{n^n}{\prod_{i=1}^d (na_i)^{na_i}} = n\log n - \sum_{i=1}^{d} na_i \log(na_i) \\ &= n\left(\log n - \sum_{i=1}^{d} a_i(\log n + \log a_i)\right) \\ &= n\left(\log n - \log n\sum_{i=1}^{d} a_i - \sum_{i=1}^{d} a_i \log a_i\right) = -n\sum_{i=1}^{d} a_i \log a_i. \qquad (3.3) \end{aligned}$$

Combining (3.1), (3.2), and (3.3) yields

$$\begin{aligned}
\log P(S^{(d)}(n) = n\alpha, N = na) &= -\frac{n}{2}\sum_{i=1}^{d} a_i \left(2\log a_i + (1+\frac{\alpha_i}{a_i})\log(1+\frac{\alpha_i}{a_i}) + (1-\frac{\alpha_i}{a_i})\log(1-\frac{\alpha_i}{a_i})\right) \\
&\qquad -n\log d \\
&= -\frac{n}{2}\sum_{i=1}^{d}\Bigg(2a_i\log a_i + (a_i+\alpha_i)(\log(a_i+\alpha_i) - \log(a_i)) \\
&\qquad +(a_i-\alpha_i)(\log(a_i-\alpha_i) - \log(a_i))\Bigg) - n\log d \\
&= -\frac{n}{2}\sum_{i=1}^{d}\Big((a_i+\alpha_i)\log(a_i+\alpha_i) + (a_i-\alpha_i)\log(a_i-\alpha_i)\Big) - n\log d.
\end{aligned}$$

This gives the expression in (2.1). To determine the criterion on the coefficients a_i, note that the maximum of $P(S^{(d)}(n) = n\alpha, N = na)$ is attained at the same point as the minimum of

$$f_\alpha(a) = \sum_{i=1}^{d}\Big((a_i+\alpha_i)\log(a_i+\alpha_i) + (a_i-\alpha_i)\log(a_i-\alpha_i)\Big).$$

It is easy to see that

$$\nabla f_\alpha(a) = 0 \iff \log(a_i^2 - \alpha_i^2) = \log(a_d^2 - \alpha_d^2)\,\forall 1 \le i \le d.$$

This shows that the expression in (2.1) with conditions (2.2) and (2.3) is indeed the large deviations rate function for d-dimensional simple random walk, so the proof is complete since, as shown for instance in Borovkov and Mogulskii (1999), that function also dictates the moderate deviations behavior of the random walk.

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