The return probability for 3D lattices

The return probability (to the origin) is given by

$$\widehat{F}_{u=1}(x_0,x_0) = 1 - \frac{1}{\widehat{p}_{u=1}(x_0,x_0)} = 1 - \frac{1}{\widehat{p}_{u=1}(0,0)}. \tag{1}$$

By definition,

$$\widehat{p}_{u=1}(0,0) = 1 + \sum_{N=1}^{\infty} p_N(0,0).$$

We showed earlier that ${}^d p_N\left(\overrightarrow{0}\right) \sim \frac{c_d}{N^{d/2}}$.Thus, for $d = 1, 2$ $\widehat{p}_{u=1}(0,0) = \infty$ and $\widehat{F}_{u=1}(x_0,x_0) = 1$. For $d \geq 3$, $\widehat{p}_{u=1}(0,0)$ is finite and hence, $\widehat{F}_{u=1}(x_0,x_0) < 1$.

Using the tools we developed earlier it is possible to calculate the return probability for a few types of lattice in three-dimensions.

$$p_N\left(\overrightarrow{x},\overrightarrow{0}\right) = \left(\frac{1}{2\pi}\right)^3 \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \widetilde{f}^N\left(\overrightarrow{k}\right) e^{-i\overrightarrow{k}\cdot\overrightarrow{x}} d^3k.$$

Multiplying both sides by u^N and summing over N one finds,

$$\begin{aligned}
\widehat{p}_u\left(\overrightarrow{x},\overrightarrow{0}\right) &= \sum_{N=0}^{\infty} u^N p_N\left(\overrightarrow{x},\overrightarrow{0}\right) = \left(\frac{1}{2\pi}\right)^3 \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \sum_{N=0}^{\infty}\left[u\widetilde{f}\left(\overrightarrow{k}\right)\right]^N e^{-i\overrightarrow{k}\cdot\overrightarrow{x}} d^3k \\
&= \left(\frac{1}{2\pi}\right)^3 \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{1}{1-u\widetilde{f}\left(\overrightarrow{k}\right)} e^{-i\overrightarrow{k}\cdot\overrightarrow{x}} d^3k.
\end{aligned}$$

In particular,

$$\widehat{p}_{u=1}\left(\overrightarrow{0},\overrightarrow{0}\right) = \left(\frac{1}{2\pi}\right)^3 \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{1}{1-\widetilde{f}\left(\overrightarrow{k}\right)} d^3k. \tag{2}$$

For simple cubic lattice,

$$f_{SC}\left(\overrightarrow{\Delta x}\right) = \frac{1}{6}\begin{pmatrix} \delta(\Delta y)\,\delta(\Delta z)\sum_{s_i=\pm1}\delta(\Delta x - s_i) \\ +\delta(\Delta z)\,\delta(\Delta x)\sum_{s_i=\pm1}\delta(\Delta y - s_i) \\ +\delta(\Delta y)\,\delta(\Delta x)\sum_{s_i=\pm1}\delta(\Delta z - s_i) \end{pmatrix},$$

$$\widetilde{f}_{SC}\left(\overrightarrow{k}\right) = \frac{\sum_{i=1}^{3}\cos(k_i)}{3}.$$

For BCC lattice,

$$f_{BCC}\left(\overrightarrow{\Delta x}\right) = \frac{1}{8}\sum_{s_i,s_j,s_l=\pm1}\delta(\Delta z - s_l)\,\delta(\Delta y - s_j)\,\delta(\Delta x - s_i),$$

$$\widetilde{f}_{BCC}\left(\overrightarrow{k}\right) = \prod_{i=1}^{3}\cos(k_i).$$

For FCC lattice,

$$f_{FCC}\left(\overrightarrow{\Delta x}\right)=\frac{1}{12}\left(\begin{array}{c}\sum\limits_{s_i,s_j=\pm1}\delta\left(\Delta x\right)\delta\left(\Delta y-s_j\right)\delta\left(\Delta z-s_i\right)\\+\sum\limits_{s_i,s_j=\pm1}\delta\left(\Delta y\right)\delta\left(\Delta x-s_j\right)\delta\left(\Delta z-s_i\right)\\+\sum\limits_{s_i,s_j=\pm1}\delta\left(\Delta z\right)\delta\left(\Delta y-s_j\right)\delta\left(\Delta x-s_i\right)\end{array}\right),$$

$$\widetilde{f}_{FCC}\left(\overrightarrow{k}\right)=\frac{1}{6}\sum_{i=1,j=1,i\neq j}^{3}\cos(k_j)\cos\left(k_i\right).$$

(*Note that the sum includes $\cos(k_1)\cos\left(k_2\right)$ and $\cos(k_2)\cos\left(k_1\right)$ so when writing explicitly it looks like $\frac{1}{3}\left(\cos(k_1)\cos\left(k_2\right)+\cos(k_1)\cos\left(k_3\right)+\cos(k_2)\cos\left(k_3\right)\right)$)

Numerical calculations of the integral in equation (2) yields for the different lattice types:

$$\begin{aligned}{}^{SC}\widehat{p}_{u=1}\left(\overrightarrow{0},\overrightarrow{0}\right)&=1.516,\\{}^{BCC}\widehat{p}_{u=1}\left(\overrightarrow{0},\overrightarrow{0}\right)&=1.393,\\{}^{FCC}\widehat{p}_{u=1}\left(\overrightarrow{0},\overrightarrow{0}\right)&=1.344.\end{aligned}$$

The return probabilities are:

$$\begin{aligned}{}^{SC}\widehat{F}_{u=1}\left(\overrightarrow{0},\overrightarrow{0}\right)&=0.3405,\\{}^{BCC}\widehat{F}_{u=1}\left(\overrightarrow{0},\overrightarrow{0}\right)&=0.282,\\{}^{FCC}\widehat{F}_{u=1}\left(\overrightarrow{0},\overrightarrow{0}\right)&=0.256.\end{aligned}$$

The larger is the number of nearest neighbors the larger is the number of escape routes. Hence, the smaller is the return probability. (note that for the SC lattice there are 6 nearest neighbors, for the BCC there are 8 n.n. and for the FCC there are 12 n.n.)

Non Identical Independent Steps

It is possible that the steps of the random walk are not identical but they are independent. In this case, there are N transition PDFs, $p_m\left(x\right)$ and N corresponding characteristic functions, $\widetilde{p}_m\left(k\right)$ (one for each step). Independence of the steps implies

$$\widetilde{P}_N\left(k\right)=\prod_{m=1}^{N}\widetilde{p}_m\left(k\right),\tag{3}$$

or

$$\ln\left(\widetilde{P}_N\left(k\right)\right)=\sum_{m=1}^{N}\ln\left(\widetilde{p}_m\left(k\right)\right)=\sum_{m=1}^{N}\sum_{l=1}^{\infty}\frac{\left(-ik\right)^l}{l!}c_{m,l}.\tag{4}$$

$c_{m,l}$ is the $l'th$ cumulant of the $m'th$ step. Assuming that the walk is unbiased, i.e., the average of each of the steps is zero, we can write eq. (4) as:

$$\ln\left(\widetilde{P}_N\left(k\right)\right)=\sum_{m=1}^{N}\sum_{l=2}^{\infty}\frac{\left(-ik\right)^l}{l!}c_{m,l}=\sum_{l=2}^{\infty}\frac{\left(-ik\right)^l}{l!}\sum_{m=1}^{N}c_{m,l}=\sum_{l=2}^{\infty}\frac{\left(-ik\right)^l}{l!}C_{N,l}.\tag{5}$$

Here we defined

$$C_{N,l} \equiv \sum_{m=1}^{N} c_{m,l}, \tag{6}$$

which is the $l'th$ cumulant of the position after N steps. Eq. (6) reflects the additivity of the cumulants when the steps are independent. When the steps are weakly non identical, i.e., the sum of the cumulants of the independent steps is finite, the usual cumulant may be replaced by the average cumulant and the CLT holds. In this case,

$$\overline{c}_l = \lim_{N\to\infty} \frac{1}{N} \sum_{m=1}^{N} c_{m,l}. \tag{7}$$

If $\overline{c}_l$ is positive and finite $C_{N,l} \sim N\overline{c}_l$ for $N \to \infty$. The fluctuations around this value decrease as N increases. Remember that we showed

$$\ln\left(\widetilde{P}_N(k)\right) = -\frac{k^2 N}{2!}\overline{c}_2 + i\frac{k^3 N}{3!}\overline{c}_3 + \frac{k^4 N}{4!}\overline{c}_4 + ... \tag{8}$$

Changing variables according to $w = k\sqrt{N\overline{\sigma^2}}$ and $\zeta = \frac{x}{\sqrt{N\overline{\sigma^2}}}$ yields

$$\ln \widetilde{\Phi}_N(w) \sim -\frac{w^2}{2} + i\frac{w^3}{3!\sqrt{N}}\lambda_3 + \frac{w^4}{4!N}\lambda_4 + ... \tag{9}$$

where

$$\lambda_l = \frac{\overline{c}_l}{\left(\sqrt{\overline{\sigma^2}}\right)^l}. \tag{10}$$

$\sqrt{\overline{\sigma^2}}$ sets the scale (the sqrt of the average variance, AKA as the standard deviation). From eq. (9), it's obvious that the PDF of ζ is a standard normal distribution; therefore, the PDF of $x/\sqrt{N}$ is a Gaussian with variance equal to the average variance.

In general, if we define $w = kC_{N,2}^{1/2}$ and $\zeta = \frac{x}{C_{N,2}^{1/2}}$ we find

$$\ln \widetilde{\Phi}_N(w) \sim -\frac{w^2}{2} + i\frac{w^3}{3!}\frac{\overline{c}_3}{\overline{c}_2^{3/2}}\lambda_3 + ..., \tag{11}$$

which implies that the CLT holds if

$$\lim_{N\to\infty} \frac{\overline{c}_l}{\overline{c}_2^{l/2}} = 0 \text{ for } l \geq 3.$$

Example 1

Consider a RW with non-identical steps which are rescaled from a common PDF of $\widetilde{\Delta x}$.

$$X_N = \sum_{m=1}^{N} \Delta x_m = \sum_{m=1}^{N} a_m \widetilde{\Delta x}_m,$$

where a_m is any function of m and the $\widetilde{\Delta x}_m$s are i.i.d. variables with zero mean and all cumulants finite. If we denote as c_l the $l'th$ cumulant of the common variable $\widetilde{\Delta x}$, we can express the $l'th$ cumulant of the position after N steps as:

$$C_{N,l} = c_l \sum_{m=1}^{N} a_m^l.$$

We can express the cumulants of the rescaled variables as

$$\frac{C_{N,l}}{C_{N,2}^{l/2}}=\frac{c_l}{c_2^{l/2}}\frac{\sum\limits_{m=1}^{N}a_m^l}{\left(\sum\limits_{m=1}^{N}a_m^2\right)^{l/2}}=\lambda_l A_{N,l},$$

where

$$\lambda_l=\frac{c_l}{c_2^{l/2}}\text{ and }A_{N,l}=\frac{\sum\limits_{m=1}^{N}a_m^l}{\left(\sum\limits_{m=1}^{N}a_m^2\right)^{l/2}}.$$

We showed that if $\lim_{N\to\infty}A_{N,l}\to 0$ for $l\geq 3$, the CLT holds for the RW. In what follows, we will consider several examples with specific dependence of the a_ms on m.

Example: Power-law growing/decaying steps

Consider the case of

$$a_m=m^{\alpha},\text{ and }c_{l>1}=1\text{ (for simplicity).}$$

We find the second cumulant of the displacement after N steps to be

$$C_{N,2}=c_2\sum_{m=1}^{N}a_m^2=\sum_{m=1}^{N}m^{2\alpha}.$$

We can distinguish between several cases,

$$C_{N,2}\sim\begin{cases}N^{2\alpha+1} & \alpha>-\frac{1}{2}\\ \ln(N) & \alpha=-\frac{1}{2}\\ \varsigma(-2\alpha) & \alpha<-\frac{1}{2}\end{cases},$$

where

$$\varsigma(z)=\sum_{n=1}^{\infty}\frac{1}{n^z},$$

is the Reimann zeta function.

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The zeta function is used in number theory due to Euler's identity

$$\varsigma(z)=\sum_{n=1}^{\infty}\frac{1}{n^z}=\prod_{prime\geq 2}\frac{1}{1-1/p^z}.$$

Note that the divergence of the zeta function for $z=1$ for which the product becomes

$$\varsigma(1)=\prod_{prime\geq 2}\frac{p}{p-1},$$

implies that there is an infinite number of prime numbers.

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Back to the RW, higher cumulants are expressed as

$$C_{N,l}\sim\begin{cases}N^{l\alpha+1} & \alpha>-\frac{1}{l}\\ \ln(N) & \alpha=-\frac{1}{l}\\ \varsigma(-l\alpha) & \alpha<-\frac{1}{l}\end{cases}.$$

The first order correction to the CLT depends on the third cumulant. Therefore, we distinguish between the different cases:

$$\underline{\alpha > -1/3}$$

$$\frac{C_{N,3}}{C_{N,2}^{3/2}} \sim \frac{N^{3\alpha+1}}{\left(N^{2\alpha+1}\right)^{3/2}} = \frac{1}{\sqrt{N}} \text{ which vanishes in the limit of } N \to \infty.$$

The higher scaled cumulants are given by

$$\frac{C_{N,l}}{C_{N,2}^{l/2}} \sim \frac{1}{\left(N^{2\alpha+1}\right)^{l/2}} \left\{N^{l\alpha+1} \quad \text{or} \quad \ln(N) \quad \text{or } \varsigma(-l\alpha) \text{ according to } \alpha\right\}$$

For $l > 3$ all the cumulants vanish as $N \to \infty$.Therefore, the CLT for $y = X_N/\sqrt{C_{N,2}} = X_N/N^{\alpha+1/2}$ holds.

$$\underline{\alpha = -1/3}$$

$$\frac{C_{N,3}}{C_{N,2}^{3/2}} \sim \frac{\ln(N)}{N^{3\alpha+3/2}} = \frac{\ln(N)}{N^{1/2}} \text{ which vanishes in the limit of } N \to \infty.$$

$$\underline{-1/2 < \alpha < -1/3}$$

$$\begin{aligned} \frac{C_{N,3}}{C_{N,2}^{3/2}} &\sim \frac{\varsigma(-3\alpha)}{N^{3\alpha+3/2}} \text{which vanishes in the limit of } N \to \infty. \\ \frac{C_{N,l}}{C_{N,2}^{l/2}} &\sim \frac{\varsigma(-l\alpha)}{N^{l\alpha+l/2}} \text{which vanishes in the limit of } N \to \infty \text{ for } l > 3. \end{aligned}$$

$$\underline{\alpha = -1/2}$$

$$\frac{C_{N,l}}{C_{N,2}^{l/2}} \sim \frac{\varsigma(-l\alpha)}{(\ln(N))^{l/2}} \text{which vanishes in the limit of } N \to \infty \text{ for } l \geq 3.$$

$$\underline{-1 < \alpha < -1/2}$$

$$\begin{aligned} C_{N,2} &\sim \varsigma(-2\alpha) \\ \frac{C_{N,l}}{C_{N,2}^{l/2}} &\sim \frac{\varsigma(-l\alpha)}{\left(\varsigma(-2\alpha)\right)^{l/2}} \text{which is finite in the limit of } N \to \infty \text{ for } l \geq 3. \end{aligned}$$

Therefore, despite having a bounded mean squared displacement (MSD) the tails are not bounded.