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Relating Microscopic and Macroscopic Parameters for a 3-Dimensional Random Walk*

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Abstract. We consider a particle undergoing a discrete random walk with killing. We relate the microscopic transition and killing probabilities to these same parameters at a macroscopic level. We find the appropriate scaling laws.

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Introduction

Consider the unit cube $\mathbb{C}$ in three-dimensional space. For any value of $n = 0, 1, 2, \ldots$ we partition this unit cube $\mathbb{C}$ into 8^n "little cubes" denoted by $\mathbb{C}_n$. These cubes are obtained by successive bisections of each of the sides of the unit cube and the sides of each $\mathbb{C}_n$ has length $(1/2)^n$.

For a fixed value of n we consider a 2-step Markov process with state space given by the 8^n "little cubes" $\mathbb{C}_n$. The evolution of a "particle" in this discrete time process is as follows: at each site there is a probability v_n of being killed. If a particle is not killed at a site $\mathbb{C}_n$, then it makes a transition to one of its six neighbors with probabilities that depend on the way in which the particle arrived at the present state. These probabilities are f_n, b_n and s_n and they give the probability of a "forward transition," i.e. one that preserves the direction of the last transition, a "backward transition." i.e. one that reverses this direction or finally a "sideways transition." where a ninety degree turn (in any one of the four possible directions) with respect

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to the last transition is taken. We have a 2-step Markov process since the transitions from every cube depend on the present and previous states.

We arrange these quantities so that

$$f_n + 4s_n + b_n = 1.$$

Notice that f_n, b_n, s_n are *conditional* transition probabilities, so that for instance the probability of a transition into one face of a "little cube" $\mathbb{C}_n$ and out through its opposite face is given by the product $(1 - v_n)f_n$. Also notice that we can consider (v_n, f_n, s_n) as *independent* quantities, with b_n determined by the latter two.

Micro and Macroscopic Parameters

Think now of one face of the unit cube as being made up of $2^n \times 2^n$ faces of some of the "little cubes" $\mathbb{C}_n$. To fix ideas position the cube in such a way that this is the bottom face. With probability 2^{-2n} pick one of the "little faces" that make up this bottom face and "push up" a particle into the corresponding little cube $\mathbb{C}_n$. Now let this particle evolve according to the 2-step Markov process described above. This particle will wander around inside the unit cube until it will eventually surface at some of the exposed faces of the "little cubes" $\mathbb{C}_n$. This exit face could be either the top face of the unit cube $\mathbb{C}$, or one of the side faces, or the bottom face. Finally there is the possibility that the particle would be killed somewhere along the way and would never make it to the surface of the unit cube. These four probabilities are illustrated by the paths α, β, γ and δ respectively in the figure below.

Summing over the equally probable "little faces" on the bottom face that serves as launching path for our particle we can thus talk about the probability that a particle that was "pushed up" from the bottom face is killed inside the unit cube. Conditional on not being killed one can also talk about the probability of a forward, sideways or backward transition within the unit cube, i.e. the probability of emerging at the top face, one of the lateral faces or the bottom face.

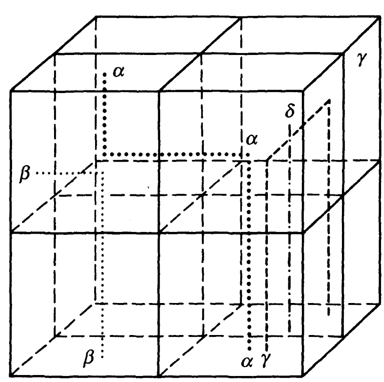

Fig. 1

These quantities depend on (v_n, f_n, s_n) and we denote them by $(v^{(n)}, f^{(n)}, s^{(n)}, b^{(n)})$. Once again we have—for symmetry reasons—

$$f^{(n)} + 4s^{(n)} + b^{(n)} = 1,$$

and we thus concentrate on

$$v^{(n)}(v_n, f_n, s_n), \quad f^{(n)}(v_n, f_n, s_n) \quad \text{and} \quad s^{(n)}(v_n, f_n, s_n).$$

We refer to (v_n, f_n, s_n) as the "microscopic" parameters and to $(v^{(n)}, f^{(n)}, s^{(n)})$ as the resulting "macroscopic" parameters.

We are now ready to state the problem considered in this paper.

Given four quantities

$$v, f, s, b$$

normalized by the condition

$$f + 4s + b = 1,$$

how should one choose the "microscopic" parameters (v_n, f_n, s_n) in such a way that the resulting "macroscopic" parameters $(v^{(n)}, f^{(n)}, s^{(n)})$ would converge to (v, f, s) as n goes to infinity?

It is intuitively clear that if the limiting values of $1 - v^{(n)}$ and $f^{(n)}$ are to be nonzero then the values of v_n and f_n should approach zero and one respectively. Much less clear is the issue of the rate at which these quantities should approach these limits.

One can make some kind of handwaving argument to advance the ansatz that the correct choice is given by

$$v_n = v/2^n,$$

$$1 - f_n = \frac{1-f}{2n},$$

$$s_n = s/2^n.$$

The purpose of this paper is to provide a "corrected version" of this ansatz. We will show the existence of three functions

$$\tilde{v}(v, f, s), \quad \tilde{f}(v, f, s), \quad \tilde{s}(v, f, s)$$

which are analytic in a neighborhood of $v = 0$, $f = 1$, $s = 0$, and such that if we put

$$v_n = \tilde{v}/2^n$$

$$f_n = 1 - \frac{1-\tilde{f}}{2^n}$$

$$s_n = \tilde{s}/2^n,$$

we get

$$\lim_{n\to\infty} v^{(n)}(v_n, f_n, s_n) = v,$$

$$\lim_{n\to\infty} f^{(n)}(v_n, f_n, s_n) = f,$$

$$\lim_{n\to\infty} s^{(n)}(v_n, f_n, s_n) = s.$$

Moreover it will turn out that, around $v = 0$, $f = 1$, $s = 0$ we have

$$\tilde{v} = v + \text{higher order terms},$$
$$\tilde{f} = f + \text{higher order terms},$$
$$\tilde{s} = s + \text{higher order terms}.$$

If the higher order terms were absent then the original ansatz would have been correct. The difference between $\tilde{v}, \tilde{f}, \tilde{s}$ and its linearized part at the origin, (v, f, s), gives the "correction" referred to above. We have been unable to obtain a closed from expression for $\tilde{v}, \tilde{f}, \tilde{s}$ and we give an exact power series expansion up to order two. We have, however, obtained the analytical tools that would allow anyone to compute more terms in these expansions if this were deemed desirable.

The Doubling Formula

The crucial step in this paper is given in the expressions below. They relate the killing probability as well as the conditional forward and sideways transition probabilities of a "little cube" $\mathbb{C}_{n+1}$ to the corresponding quantities for the "big cube" $\mathbb{C}_n$ made up of eight identical copies of $\mathbb{C}_{n+1}$.

By a careful consideration of the geometrical setup one can write down a system of linear equations, the "forward" equations for the 2-step Markov process in question and conclude after some laborious computation that if (v, f, s) are the common values of the parameters for each $\mathbb{C}_{n+1}$, then the new values for a cube $\mathbb{C}_n$ are given by the rather compact expressions

$$v_{\text{new}} = 2v + \frac{v^2}{(2s+b)(1-v)-1},$$

$$f_{\text{new}} = \frac{w(2s^2w + 3fsw + f^2w - fw + f)^2}{\begin{array}{l}(4sw + 2fw - w - 2s - f + 1)(1 - 10s^2w^2 - 7fsw^2 \\ \quad + 7sw^2 - f^2w^2 + 2fw^2 - w^2 - sw)(5sw + fw - w + 1)\end{array}},$$

$$s_{\text{new}} = \frac{s(4sw + 2fw - w + 1)^2}{2(4sw + 2fw - w - 2s - f + 1)(5sw + fw - w + 1)}.$$

In the last two expressions we have used

$$w \equiv 1 - v$$

to render the formulas a bit simpler. It is quite likely that these formulas can be arrived at by a skillful "summation over paths." This is not hard to do in some simple cases, but in general we find that solving the equations mentioned above is the best way to get a closed form solution. We have obtained these compact forms of the solution with help from Vaxima, a symbol manipulator at Berkeley.

We are particularly interested in the behavior around the *trivial case* $v = 0$, $s = 0$, $f = 1$, i.e. a case where all the paths originating on one face emerge on the opposite face. This makes it natural to use as variables the quantities

$$v, s \text{ and } g \equiv 1 - f.$$

With the understanding that v_{new} and s_{new} retain their original meaning and that

$$g_{\text{new}} \equiv 1 - f_{\text{new}},$$

we obtain

$$v_{\text{new}} = 1 - \frac{(1-v)(4sv - 2gv + v - 2s + g - 1)}{2sv - gv - 2s + g - 1},$$

$$g_{\text{new}} = 1 - \frac{(1-v)(2s^2v - 3gsv + 3sv + g^2v - gv - 2s^2 + 3gs - 3s - g^2 + 2g - 1)^2}{(1 - 10s^2v^2 + 7gsv^2 - g^2v^2 + 20s^2v - 14gsv + sv + 2g^2v - 10s^2 + 7gs - s - g^2)P},$$

$$s_{\text{new}} = \frac{s(4sv - 2gv + v - 4s + 2g - 2)^2}{2P},$$

with $P \equiv (4sv - 2gv + v - 2s + g - 1)(5sv - gv - 5s + g - 1)$.

We refer to these expressions as the "doubling formula" since they relate the parameters (v, g, s) of a "little cube" to those of the "doubled" cube obtained by packing together eight copies of it.

We see below that around the value

$$v = 0, \quad g = 0, \; s = 0$$

the map $(v, g, s) \to (v_{\text{new}}, g_{\text{new}}, s_{\text{new}})$ is exactly twice the identity map, i.e. these parameters get doubled. We have, up to terms order three

$$v_{\text{new}} = 2v - v^2 - gv^2 + 2sv^2 + \cdots,$$

$$g_{\text{new}} = 2g - 2g^2 + 8gs - 20s^2 + 2g^3 - 16g^2s + 28gs^2 + 28s^3 - 16gsw + 36s^2v + gv^2 + \cdots,$$

$$s_{\text{new}} = 2s - 6s^2 - 6gs^2 + \frac{sv^2}{2} + 10s^2v - 2gsv + 30s^3 + \cdots.$$

We will denote below by T the map

$$(v, g, s) \to (v_{\text{new}}, g_{\text{new}}, s_{\text{new}})$$

introduced above. The explicit expressions given above make it obvious that T is analytic in all its variables for (v, g, s) close to $(0, 0, 0)$. T maps the origin into itself. Moreover, we have just seen that the gradient S of this map at the origin $\equiv (0, 0, 0)$ is $2I$; as a consequence the map T itself is locally invertible around the origin. Here and below when we talk about the inverse of a map we always mean a local inverse, which exists around the origin. We have been unable to obtain an explicit expression for the inverse map.

Iterating the Map T

Recall that the map T relates the parameters corresponding to cubes $\mathbb{C}_{n+1}$ to those of cubes $\mathbb{C}_n$. Therefore, if for a given n we choose values (v_n, g_n, s_n) for the individual cubes $\mathbb{C}_n$, we get that the values for the unit cube $\mathbb{C}$ $(= \mathbb{C}_0)$ are

$$T^n(v_n, g_n, s_n),$$

where the exponent denotes iteration of the map T n times.

Recall that the original problem was one of choosing (v_n, g_n, s_n) in such a way that the limit of the above expression would agree with a given value (v, g, s).

If we put, on "physical grounds,"

$$v_n = v/2^n, \quad g_n = g/2^n, \quad s_n = s/2^n,$$

i.e.

$$(v_n, g_n, s_n) = S^{-n}(v, g, s)$$

with $S \equiv 2I$, we obtain for the macroscopic parameters the expression

$$T^n S^{-n}(v, g, s).$$

This brings up the question of the existence of the limit

$$\lim_{n \to +\infty} T^n S^{-n}.$$

We will show below that this limit exists, at least for (v, g, s) close enough to the origin, and that is given by some (locally) analytic function φ which admits a (locally) analytic inverse ψ. These functions $\varphi = (\varphi_1, \varphi_2, \varphi_3)$, $\psi = (\psi_1, \psi_2, \psi_3)$ map neighborhoods of the origin in R^3 onto each other.

Therefore we have

$$\lim_{n \to \infty} T^n S^{-n} \psi = I,$$

which indicates that the ansatz made above should be changed into

$$v_n = \psi_1(v, g, s)/2^n,$$

$$g_n = \psi_2(v, g, s)/2^n,$$

$$s_n = \psi_3(v, g, s)/2^n.$$

If (v_n, g_n, s_n) are chosen in this fashion at the microscopic level, we obtain the values (v, g, s) as the limiting macroscopic parameters.

We conclude by indicating the reason for the existence of the maps φ and ψ mentioned above and by giving the first few terms of these maps explicitly as well as a general procedure for computing φ and ψ to any order required.

Intertwining Maps and "Wave" Operators

Given an analytic map T with $T(\bar{0}) = \bar{0}$ and its gradient S at the origin $\equiv \bar{0} \in R^m$, it is natural to ask two questions

a) does there exist an analytic map φ whose linear part at the origin is the identity and such that

$$T\varphi = \varphi S?$$

b) does the limit

$$\lim_{n \to \infty} T^n S^{-n}$$

exist, and if so, what is the relation to a map φ as in part a)?

The study of "intertwining maps" φ satisfying

$$T\varphi = \varphi S$$

has a venerable history. It has its origin in work of Abel, Schroeder [1], Poincaré [2], Koenigs [3], Levy [4], and has been furthered by Leau [5], Sternberg [6] and Hartman [7] among others.

The study of the expression

$$\lim_{n \to \infty} T^n S^{-n}$$

is a common occurrence in "scattering theory" where they are known as the "Moeller wave operator," see [8]. Although they have usually been considered in the case where all maps are linear, these ideas have been used also in nonlinear setups, see [9] and [10].

Without reproducing all these results here we quote the relevant portions for our purposes.

As to question a) we have, in our case, $S = 2I$. Since the three eigenvalues of S, $\lambda_1 = \lambda_2 = \lambda_3 = 2$, do not give rise to any "small divisor problem"

$$\lambda_i = \lambda_1^{n_1} \lambda_2^{n_2} \lambda_3^{n_3},$$

$$n_1 + n_2 + n_3 > 1, \quad n_i \text{ nonnegative integers,}$$

we are guaranteed the existence of an analytic φ with

$$T\varphi = \varphi S.$$

If we insist that the linear part of φ at $(0,0,0)$ be the identity map, then this φ is unique.

Question b) has, in our case, an affirmative answer too. From

$$\varphi S = T\varphi$$

we get

$$T^n = \varphi S^n \varphi^{-1}$$

and then

$$T^n S^{-n} = \varphi(S^n \varphi^{-1} S^n).$$

One can now prove rather easily that since the linear part of φ^{-1} is the identity I we get

$$\lim_{n \to \infty} S^n \varphi^{-1} S^n = I$$

and thus

$$\lim_{n \to \infty} T^n S^{-n} = \varphi.$$

The remaining task is to get the first few terms in the expression for φ.

We could use the functional equation

$$T\varphi = \varphi S$$

or even better the equation

$$S\psi = \psi T$$

satisfied by $\psi = \varphi^{-1}$. Once we get an approproximation to ψ we can deduce one for φ.

Using the second functional equation we get for ψ the expansion

$$\psi(v, g, s) = \left(v + \frac{v^2}{2} + \cdots, g + 10s^2 - 4gs + g^2 + \cdots, s + 3s^2 + \cdots \right).$$

From here it follows that φ has an expansion

$$\varphi(v, g, s)\left(v - \frac{v^2}{2} + \cdots, g - 10s^2 + 4gs - g^2 + \cdots, s - 3s^2 + \cdots \right).$$

Both expansions are accurate up to order two. It is, of course, possible to carry out these computations to higher order of accuracy.

In the much simpler two-dimensional case *without killing*, i.e. $v \equiv 0$, one can find in [11] expressions for φ and ψ up to order six, along with comparisons between this approximation to φ and those given by the expression $T^n S^{-n}$ for increasing values of n.

References

1. Schroder, E.: Über iterierte Funktionen. Math. Ann. **2**, 317–365 (1870)
2. Poincaré, H.: Oeuvres, Vol. 1, pp. XCIX–CV of Thesis
3. Koenigs, G.: Recherches sur les intégrales de certaines équations fonctionnelles. Ann. Sci. École Norm. Sup. Supp. 3–41 (1984)
4. Lévy, P.: Fonctions à croissance régulière et itération d'ordre fractionnaire. Ann. Mat. Pura Appl **5**, 269–298 (1928)
5. Leau, L.: Etude sur les equations fonctionelle a une ou plusieurs variables. Annales de la Faculte des Sciences de Toulouse 11, E.1–E.110 (1987)
6. Sternberg, S.: Local contractions and a theorem of Poincaré, Am. J. Math. **79**, 809–824 (1957)
7. Hartman, P.: Ordinary differential equations. New York: Wiley 1964
8. Kato, T.: Perturbation theory of linear operators. Berlin, Heidelberg, New York: Springer 1966
9. Nelson, E.: Topics in dynamics. Princeton, NJ: Princeton University Press 1968–1969
10. Grünbaum, F. A.: On the existence of a "wave operator" for the Boltzmann equation, Bull. Am. Math. Soc. **78**, 759–762 (1972)
11. Grünbaum, F. A.: Renormalization of exit probabilities and a theorem of Poincaré. To appear in Physics Letters A

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