Anomalous Diffusion on Random Graphs

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We show that anomalous diffusion can result when the steps of a random walk are not statistically independent. We present an algorithm that counts all the possible paths of particles diffusing on random graphs with arbitrary degree distribution. Using this to calculate the mean square displacement, we show that in sharp contrast to continua, random walks on random graphs can exhibit anomalous behavior and yet have well-defined and predictable properties.

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It is well known that a random walk on a continuous medium leads to a mean square displacement ⟨x²⟩ that is linear in time as long as there are no infinitely large steps and all steps are statistically independent. Lévy showed that anomalous diffusion results when the former assumption is violated. In this paper we show that anomalous diffusion results when the latter assumption is violated but the former remains, by considering random walks on random graphs.

Random graphs have been very successfully used to describe many diverse systems. For example, the spreading of diseases through a population has been modelled where people are the vertices and contact between them the edges [1, 2]. The internet can be thought of as a graph with web sites as vertices and links as edges, leading to estimates of the number of clicks to surf between any two random sites and other quantities of interest [3, 4]. In general, any system with interacting parts, which encompasses a vast array of diverse systems, can be mapped onto a graph [5].

Along with to statics, dynamic properties of random graphs are of interest for many cases like protein folding [6] and glassy relaxation [7]. In this paper we consider particles diffusing along the edges of a random graph and develop a method for calculating diffusion on a random graph using an algorithm that counts all the paths.

The following is a brief introduction to graph theory. For a more comprehensive overview see, for example, Godsil and Royle [8]. Graphs consist of two sets: vertices, which are points, and edges, which join two vertices. In more mathematical terms, define for some index set I, the vertex set

\[ V = \{ v_i \mid i \in I \}. \]

Then, define the edge set as a subset of the pairs of all vertices

\[ E = \{ (v_j, v_k) \mid v_j, v_k \in V \} \subseteq V \times V. \]

These two sets can be thought of as points and lines in a plane as in Figure 1. The pairs of vertices defining an edge are called endpoints of the edge. There are no real restrictions on the sets of vertices and edges, making graphs very general constructions.

Like any field, graph theory has its own lingo so here are some definitions. The degree of a vertex is the number of edges with at least one endpoint at the vertex. The degree distribution \( p(k) \) is the probability that a randomly selected vertex will have degree \( k \). Two vertices are adjacent if there is an edge joining them, i.e., in Figure 1, vertices 1 and 4 are adjacent but 1 and 2 are not. A path or walk on a graph is a set of edges connecting two vertices. For example, in Figure 1 paths from 1 to 2 would be the the set of edges \( \{(1,4),(4,2)\} \) or \( \{(1,4),(4,3),(3,4),(4,2)\} \).

Now, we have enough definitions to consider why it is possible for a random graph to violate the assumption that all steps of a walk are independent. Consider the graph in Figure 1. There are three vertices with one edge and one vertex with three edges. Thus, the degree distribution is

\[ p(k) = \begin{cases} \frac{3}{4} & k = 1 \\ \frac{1}{4} & k = 3 \\ 0 & \text{otherwise} \end{cases} \]

Next, put a walker on that graph that can move from vertex to vertex along the available edges. For a walker’s first step there is a probability \( p(k) \) that it will have \( k \) choices. However, for the second step this is not necessarily the case. Still looking at the graph in Figure 1, a walker starting at vertex 1,
2, or 3 will end up at vertex 4 after one step where it will have three choices of edges on which to leave. A walker starting at vertex 4 can go to 1, 2, or 3 where it will have one choice of edges on which to leave. Thus, there are a total of six nearest neighbors, one each from vertices 1, 2, and 3 and three from vertex 4, and the degree distribution for them, \( q(k) \), is

\[
q(k) = \begin{cases}
\frac{3}{6} = \frac{1}{2} & k = 1 \\
\frac{3}{6} = \frac{1}{2} & k = 3 \\
0 & \text{otherwise}.
\end{cases}
\] (4)

Thus, since \( p(k) \neq q(k) \) the degree distribution is a function of the number of steps taken. This means that the number of choices available to a walker on a graph will depend on how far it has gone. Therefore, the assumption that all steps are uncorrelated is violated in this graph, and it can be violated generally in graphs. Note that it is not necessarily violated; for example, in a graph where all vertices have the same degree, called a regular graph, \( p(k) \) and \( q(k) \) are the same.

Moving on, some more tools for dealing with graphs will be introduced. First, define \( d(\mu, \nu) \) to be the distance between two vertices \( \mu \) and \( \nu \) which is the size of the smallest set of edges making a path starting at \( \mu \) and ending at \( \nu \). For example, in Figure 1, \( d(1, 2) = 2 \) and \( d(1, 4) = 1 \). Unless otherwise noted, all distances mentioned henceforth refer to this graph distance.

Next, define the adjacency matrix \( A \) of the graph \( G = (V, E) \) to be a square \( |V| \times |V| \) matrix with \( A_{\mu \nu} \) equal to the number of edges joining the vertices \( \mu \) and \( \nu \). Note that so long as there are no edges that connect a vertex to itself, i.e. loops, the diagonal elements of \( A \) must be zero, and an edge connecting \( \mu \) to \( \nu \) also connects \( \nu \) to \( \mu \) so \( A \) is symmetric.

As an example, consider the graph in Figure 2 which has adjacency matrix

\[
A = \begin{pmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
1 & 1 & 1 & 0
\end{pmatrix}.
\] (5)

The adjacency matrix of a graph can be used to count all paths on the graph of a given length. By definition the element \( A_{\mu \nu} \) gives the number of paths of length one from vertex \( \mu \) to \( \nu \). It can be shown by induction that \( (A^2)_{\mu \nu} \) gives the exact number of paths of length 2 from \( \mu \) to \( \nu \) \([8]\). For example, looking at the graph in Figure 3 the number of paths of length exactly two between any two vertices are given by the elements of

\[
A^2 = \begin{pmatrix}
1 & 1 & 1 & 0 \\
1 & 1 & 1 & 0 \\
1 & 1 & 1 & 0 \\
0 & 0 & 0 & 3
\end{pmatrix}.
\] (6)

The reader is encouraged to verify this by inspection. Note that edges can be traversed more than once and are multidirectional.

Consider the regular graph in Figure 2. A random walk on this graph is just the well-known drunkard’s walk with periodic boundary conditions which is not anomalous. Let \( \langle x^2(n) \rangle \) denote the average distance squared as a function of \( n \), where \( n \) is the number of steps taken and \( x \) is the distance measured from some starting vertex on the graph. One way to calculate \( \langle x^2(n) \rangle \) is to choose some starting vertex and count the fraction of paths of length \( n \) that are only a distance \( m < n \) away from the start, and then average over all possible starting vertices. Call this quantity \( p_m^n \). Looking at the drunkard’s walk graph, Figure 2 choose any vertex as the start since they are all equivalent. Then, there are two paths of length 1, one step clockwise and one step counterclockwise, both of which are distance 1 away from the start, so \( p_m^1 = \delta_m^1 \). There are four paths of length 2 of which two are one step out and one step back, giving a distance of 0, and two are two steps out clockwise or counterclockwise, giving distance 2. So \( p_m^2 \) is given by

\[
p_m^2 = \begin{cases}
\frac{1}{2} & m = 0 \\
\frac{1}{2} & m = 2 \\
0 & \text{otherwise}.
\end{cases}
\] (7)

In general, as the number of steps increases \( p_m^n \) will converge to a binomial distribution leading to the standard result

\[
\langle x^2(n) \rangle = \sum_m m^2 p_m^n = Dn,
\] (8)

where \( D \) is the diffusion coefficient \([3]\).

The central limit theorem says that changing the step size of the above walk only changes the diffusion coefficient, not the linear dependence on \( n \). Thus, if the dependence on \( n \) is
the only quantity of interest, graphs can be used to calculate it even though they ignore all spatial distances and only concentrate on the number of choices available at each step.

Using an approach similar to the above example, the adjacency matrix can be used to calculate \( p_n^m \), and hence the dependence of \( \langle x^2 \rangle \) on \( n \) for any general graph. Since the adjacency matrix \( A \) can be used to calculate the exact number of paths of a given length between any two vertices, we can enumerate all paths on the graph and find \( p_n^m \) using the following algorithm:

1. Let \( n \) be the current path length, starting with 1.
2. Raise \( A \) to the \( n \)th power.
3. Find the number of paths between any two vertices by looking at the elements of \( A^n \).
4. Keep track of the minimum distance between any two vertices by noting if this is the smallest \( n \) such that a path exists.
5. For every \( m \leq n \) find \( p_n^m \).
6. Increment \( n \) and repeat.

Once we have the distribution \( p_n^m \), all the random walk properties can be calculated. In particular, equation 8 allows the calculation of \( \langle x^2(n) \rangle \).

The method presented here for enumerating paths to calculate random walk properties reduces to just a problem of matrix multiplication. Thus, it lends itself very well to calculation by computer where efficient and easy to use matrix multiplication algorithms are readily available.

As a first test of this method, diffusion on a ring should be equivalent to the drunkard’s walk for large enough rings. The same should be true for any graph representing a regular lattice. Figure 3 shows a calculation of \( \langle x^2(n) \rangle \) using adjacency matrices as described above for a ring graph with 1000 vertices and a periodic two dimensional square lattice of size 40 by 40. From the plot it is apparent that this adjacency matrix algorithm gives the correct exponent of 1, i.e. \( \langle x^2(n) \rangle \sim n \). The slope of the lines are the diffusion coefficients which do depend on the particular system.

Now, consider some graphs which are not regular and, hence, can produce anomalous diffusion. One way to generate such graphs is to begin with a set of vertices. Next, go through all the vertices once and add edges where one endpoint of the edge is on the current vertex and the other goes to a random vertex. This guarantees that no vertices are isolated. Then, randomly connect pairs of vertices until the desired number of edges are laid down. The probability that a random vertex has \( k \) edges is given by

\[
p(k-1) = \frac{E}{k} \left( \frac{\mu}{V-1} \right)^k \left( 1 - \frac{\mu}{V-1} \right)^{E-k}, \tag{9}
\]

where \( E \) is the number of edges, and \( V \) is the number of vertices and \( \mu = 2E/V \) is the average number of edge endpoints per vertex. As the number of edges increases, \( p(k) \) in equation 9 approaches a Poisson distribution with mean \( \mu \), i.e. \( p(k) \rightarrow (\mu^k/k!) e^{-\mu} \). See Figure 4.

Once the random graph is constructed, apply the path
FIG. 6: A plot of the diffusion exponent versus the average degree for random graphs with 1800 vertices and 2000 vertices. Each are averaged over three separate realizations. Note that the anomalous exponent can be controlled by the average degree. Errors are from fitting \( x^2(n) \) to find the exponent. The lines are guides to the eye.

counting algorithm and calculate \( x^2(n) \). As an example, the result of this calculation for a graph with average degree 4 is shown in Figure 5. For comparison the values of \( x^2(n) \) are included for a ballistic walk, \( x^2(n) \sim n^2 \), and a Brownian walk \( x^2(n) \sim n \). As can be seen in Figure 5, the value of \( x^2(n) \) is somewhere between a Brownian walk and a ballistic walk so it is anomalous as expected.

For a large enough number of steps, \( x^2(n) \) of a random graph saturates because of a finite size effect. For finite random graphs such as these, there exists a finite average distance \( D_{max} \) between any two vertices which scales like the log of the number of vertices \( \log(n) \). This means that once the walker has moved a distance equal to \( D_{max} \), every new vertex to which the walker moves is still only on average a distance \( D_{max} \) away from the starting vertex. So \( x^2(n) \) approaches a constant as the number of steps approaches \( D_{max} \). Below this plateau \( x^2(n) \) follows a power law \( x^2 \sim n^\alpha \). Figure 6 shows a plot of the exponent \( \alpha \) from a power law fit for graphs with various average degrees. As can be seen from the plot, the anomalous diffusion exponent is controlled by the average degree. Also, as the average degree increases, the degree distribution approaches a Poisson distribution. At the same time, the power law for \( x^2(n) \) approaches 1.6. Thus, the exponent for a highly connected random graph with a Poisson degree distribution is 1.6.

A problem with modelling random walks with graphs is that the graph distance does not necessarily correspond to any real spatial distance. For clarification, imagine an embedding of a graph into a flat surface, i.e. random dots connected with lines on a piece of paper. Then, one can calculate \( x^2(n) \) directly by just following a large number of walkers and averaging their Euclidean distance on the surface measured from where they started as a function of time. Next, repeat this process for a new embedding of the same graph with different distances between the dots but the same connecting lines. It seems reasonable that this disorder averaging will lead to a well-defined value for the exponent. This can then be compared to the results from the adjacency matrix algorithm using the graph distance. The hope is that since both give well-defined power laws for the displacement squared, these two measurements will lead to the same power law, possibly with a different coefficient but with the same exponent. To justify this rigorously, one would have to show that the specific distribution of step sizes in the Euclidean embedding does not affect the diffusion exponent. In other words, graphs only keep track of the number of choices a walker has at each step, not the spatial distance it can go. So for the exponent calculated with the adjacency matrix algorithm to give the same results as a random walk in real space, the number of choices must be the only thing that matters.

One verification that the exponent is insensitive to the details of the spatial distances comes from our numerical calculation of the exponent for different realizations of random graphs with a given degree distribution. We find that the exponents obtained from these agree with each other within the error bars of the fit. On the other hand, the exponent changes when the degree distribution is changed. This means that it is the degree distribution, the distribution of the number of choices a walker has at each step, not the specific realization of the random graph which determines the exponent.

In conclusion, random walks on random graphs exhibit characteristics of anomalous diffusion which can be controlled by the degree distribution of the graph. Since this is drastically different from what one finds for a continuum, it seems that continua and random graphs are fundamentally different structures. Therefore, when restrictions are placed upon the ability of diffusing particles to sample their surroundings, anomalous behavior arises.

[1] C. Moore and M. E. J. Newman, Physical Review E 62, 7059 (2000).
[2] F. Liljeros, C. R. Edling, L. A. N. Amaral, H. E. Stanley, and Y. Åberg, Science 280, 98 (1998).
[3] S. Lawrence and C. L. Giles, Science 280, 98 (1998).
[4] R. Albert, H. Jeong, and A.-L. Barabási, Nature 406, 378 (2000).
[5] R. Albert and A.-L. Barabási, Review of Modern Physics 74, 47 (2002).
[6] I. M. Sokolov, J. Mai, and A. Blumen, Physical Review Letters 79, 857 (1997).
[7] A. J. Bray, and G. J. Rodgers, Physical Review B 38, 11461 (1988).
[8] C. Godsil and G. Royle, Algebraic Graph Theory, Graduate Texts in Mathematics (Springer, 2001).
[9] F. Reif, Fundamentals of Statistical and Thermal Physics (McGraw-Hill Inc., 1965).
[10] M. E. J. Newman, S. H. Strogatz, and D. J. Watts, Physical Review E 64, 026118 (2001).