FRACTALS AND FRACTAL CORRELATIONS

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Consider the object shown in Fig. 1, known as the Koch curve. It is formed by a recursive process as follows: From a line segment of length s, remove the middle third of the line segment, and in its place add two connected segments of length $s/3$. All four segments intersect at 60° or 120° in order to stay connected and are $s/3$ long. Repeat the same process to each segment to obtain 16 segments of length $s/9$, 64 segments of length $s/27$, and so on. Notice that the Koch curve has the curious property of being self-similar, meaning that it is the union of smaller copies of itself; in this case, each of the four ornamented segments is similar to the whole curve. Also note that at each step in making the curve, the length of the curve increases by a factor of 4/3. Thus in the limit of many divisions, its length is infinite. However, as Problem 1 shows, the curve has zero area in the plane. Clearly this curve is very strange; it is an example of a fractal.

We define a fractal to be a self-similar object with non-integral fractal dimension (see below). It is useful to consider two types of fractals, exact mathematical objects, such as the Koch curve, and random objects for which the statistical distribution obeys fractal scaling laws. Any particular realization of the second type of fractal is not necessarily self-similar, but a statistical average gives the same results as an exact fractal. In recent years, it has become evident that statistical fractals often occur in nature.[1]

In this column, we discuss some of the physical processes (notably those described by growth models) that generate fractal clusters of atoms or molecules. The study of these processes has increased rapidly in the last decade. We will cover some of the main themes of this research activity and also introduce some of the mathematical concepts useful for analyzing fractal clusters. A previous article[2] in this column also covered fractal aggregation. Our emphasis is somewhat different. Instead of looking in detail at the processes themselves, we will concentrate on what can be learned from the fractal properties and, in particular, discuss some interesting correlation functions.

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Fractal dimensions and long-range correlations

The fractal dimension is a way of characterizing scale changes between the object and its self-similar parts. It originally arose in mathematics to measure objects that do not behave as if they have an integral dimension. For example, as we have seen, the Koch curve exists within a finite region of two-dimensional space, but yet it has zero area and infinite length. How can we assign anything like a length or an area to this object? And if the object is neither one nor two dimensional, what is it?

The simplest way to answer these questions is the following. As in Problem 1, cover an object with boxes of varying size. We measure N, the smallest number of boxes of linear dimension r that can cover the object. As r goes to zero, if there exists a D such that N is proportional to r^{-D}, then D is the fractal dimension. Also, the generalized area, closely related to the mathematical concept of Hausdorff measure, is proportional to Nr^D. It is not difficult to see that for standard objects, such as lines and planes, the fractal dimension is the same as any other definition of dimension. For example, if we cover a line with boxes of side r, clearly we will need twice as many if the side is $r/2$, and hence $D = 1$. However, for more complicated objects D need not be an integer.

As we show below, the fractal dimension is directly related to an important physical quantity, the correlation

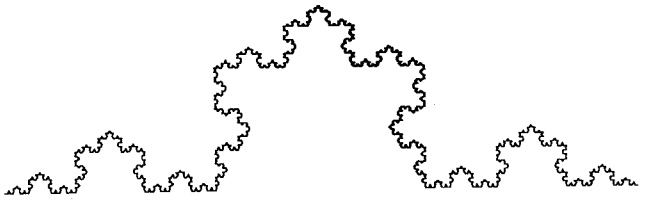

Figure 1. The Koch curve.

function $c(r,\mathbf{x})$. Given an object made up of particles, $c(r,\mathbf{x})$ is the average density of other particles at a distance r from a given particle at $\mathbf{x}$. The function $c(r,\mathbf{x})$ can be used to find much information about an object, e.g., its elasticity and how it scatters radiation. A process that distributes particles completely at random gives correlations of finite range. In this case

$$c(r,\mathbf{x}) \sim e^{-r/\xi},$$

where ξ is called the correlation length. If the object is fractal, then

$$c(r,\mathbf{x}) \sim r^{D-d},$$

where d is the dimension of the space. That is, the correlation length ξ is infinite and each part of the object influences other, distant parts. A statistical fractal is a *random* object that nevertheless has *long-range correlations*. The existence of the latter is the main reason why fractals are interesting in physics.

Box counting

The most straightforward way to calculate D for a given object is to apply the method given above. Computationally, consider an object as a list of points in d-dimensional space. Box counting amounts to partitioning a d-dimensional box containing the object into small d-dimensional boxes of linear dimension r. Count how many of the small boxes contain points from the object. This quantity is N. Since

$$N = cr^{-D},$$

where c is a constant, we have

$$\ln N = D \ln(1/r) + b,$$

where b is another constant. This equation is the equation for a line. After finding N for a series of r values, we can do a least squares fit to find an estimate for D, the slope of the line.

Correlation functions

Another method for computing the fractal dimension of an object is to use the correlation functions that we now discuss. These functions are related to the fractal dimension as follows.[3] Imagine computing the number of particles $M(R)$ that are within a distance R of the center of mass of a fractal. If we cover the whole object with one large circular box of radius R, then using box counting we have

$$N = cR^{-D} = 1,$$

so that

$$c = R^{D}.$$

Now we cover the fractal with disks of radius a that are small enough to contain just one particle, so that the number of disks $N(a)$ is the same as the number of particles $M(R)$. Thus,

$$M(R) = N(a) = [R/a]^{D}.$$

This relation is probably used more often than any other for finding D for a fractal generated by a growth process. In practice, at each stage of growth we find the number of particles M and R. Usually, instead of finding the maximum radius from the center of mass, we calculate a related quantity, the radius of gyration R_g, which is proportional to R for a fractal:

$$R_g = \sqrt{\frac{1}{M}\sum_{i=1}^{M} \mathbf{r}_i^2}, \tag{1}$$

where $\mathbf{r}_i$ is the distance to the center of mass. The sum is over the M particles in the current cluster. To obtain D, we find $R_g(M)$ and fit to $M^{1/D}$ as before. If the fractal is homogeneous, the center of mass can be replaced by any other point. In this way we have defined a correlation function $C_t(r,\mathbf{x})$, the number of particles within radius r of a given particle. That is $C_t(r,\mathbf{x})$ is the mass that surrounds point $\mathbf{x}$. The well-known[4] Grassberger–Procaccia correlation integral $C_t(r)$ is the average over $\mathbf{x}$ of $C_t(r,\mathbf{x})$.

The correlation function $c(r,\mathbf{x})$ was defined in the above as the density at radius r about $\mathbf{x}$. It is given by

$$c(r,\mathbf{x}) \sim (dM/dr)/r^{d-1} \sim r^{D-d},$$

where the numerator dM/dr is proportional to the mass and the denominator is proportional to the d-dimensional volume of a thin shell at r around $\mathbf{x}$. It is possible to compute the average of $c(r,\mathbf{x})$ over all $\mathbf{x}$ conveniently using Fourier transforms and the Wiener–Khintchine theorem,[5] but it also is relatively easy to figure it out directly.

Generalized dimensions

Although the two methods for calculating fractal dimension give the same answers for ordinary fractals, for more general objects, called multifractals, the two are different. For example, many strange attractors that arise in dynamical systems give a different answer for the two kinds of dimensions. They are related by the following generalized definition of dimension. If r is the edge length of a box and p_i is the probability that a point is in the ith box, then the generalized dimension D_q is given by the relation:

$$D_q = \lim_{r\to 0} \frac{1}{q-1} \frac{\ln \sum_{i=1}^{N} p_i^q}{\ln r}. \tag{2}$$

Box counting gives D_0, whereas correlation functions give D_2.

Fractals and growth processes

The following "chaos game" generates a fractal by a statistical process.[6] Pick a point inside an equilateral triangle. Choose an arbitrary vertex, and go half the distance to this vertex. Again choose a random vertex and go halfway to it. Keep repeating the process. After repeated iterations, what does the collection of points look like? Remarkably, this random process for growth results in an *exact* fractal called a Sierpinski gasket. It is an example of a strange attractor. Five thousand points are enough to see what the limiting behavior looks like (see Fig. 2). Unlike this example, usually statistical processes give rise to fractals that are self-similar only in the average sense discussed above. We now turn to two important physical cases.

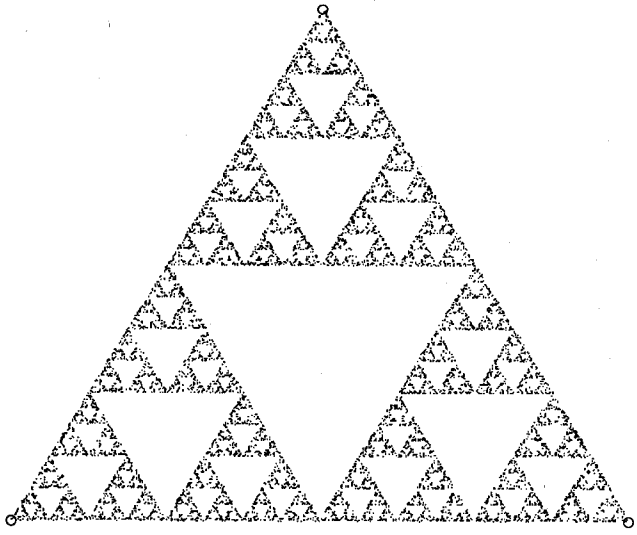

Figure 2. The result of 10,000 plays of the chaos game. Each time a point inside the triangle was chosen at random, and the distance to randomly chosen verticies was halved 20 times.

Percolation

A physical example of statistical fractals arises in percolation. This model was originally conceived to study fluid flow through rocks.[7] In one version (site percolation) the points of a lattice are populated with probability p. Populated sites correspond to spaces (pores) in rock through which fluid can flow. Neighboring populated sites are accessible to each other, as fluid can reach from one of these sites to another. The questions are whether a path across a large lattice exists, and if so, what the nature of this path is. Such a path is called a spanning cluster. In other words, we want to know whether the fluid will be able to flow through the rock.

For a square lattice the value of the percolation threshold p_c is $p_c \approx 0.592746$. For $p < p_c$, there is probability zero of a connected cluster spanning a large (infinite) lattice, but at $p = p_c$, the probability of finding such a cluster becomes nonzero. If we consider only the spanning cluster for $p > p_c$, its fractal dimension is two. Thus the spanning cluster takes up a finite fraction of the lattice. However, for $p = p_c$, the spanning cluster is a fractal with $D = 91/48 \approx 1.89$.

Another physical example modeled by percolation is gelation, such as the setting of Jello. There are particles in a fluid, forming bonds with probability p. At p_c, bonds reach across the fluid. Slightly above p_c, the substance becomes rigid. The model also has applications to epidemics and chemical reactions.[8]

It is interesting to study the fractal properties of the spanning cluster. Unfortunately, a direct use of the above model is a bit complicated because we must *find* the spanning cluster after populating the lattice. However, there is a way to generate only one spanning cluster at a time. It works by simulating an actual growth process.[9] The clusters generated by the growth process have the same correlations as those generated by site percolation. The idea is as follows: start with one populated site at the center of a lattice. Populate each neighboring site with probability p. The nearest neighbors to a lattice point (i,j) on the square lattice are the four points $(i \pm 1, j)$ and $(i, j \pm 1)$. If the neighbor is not populated, then it is blocked and can never be populated. Then generate a list of the nearest neighbors of all newly populated sites that are not already populated or blocked. Populate or block these neighbors with probability p or $1-p$, respectively. Continue this process until you have created a cluster of the desired size. If we use this method at $p = p_c$, large clusters are generated that are statistical fractals of dimension 1.89. An example is given in Fig. 3.

Diffusion-limited aggregation

Another physical model leading to fractal clusters is diffusion-limited aggregation (DLA).[3] DLA is a model of growth controlled by diffusion, in which particles perform many steps of a random walk before sticking. Start with one populated site. Far away from this site, allow another particle to perform random walk. If the new particle walks into a neighboring site of the populated site, it sticks and becomes part of the aggregate. Repeating this process for a large number of particles gives a result such as shown in Fig. 4. Realizations seem to be fractals with $D \approx 1.71$ for $d=2$ and $D \approx 2.5$ for $d=3$. One remarkable aspect about the DLA model is that many real systems appear to be well described by it. For example, crystal growth in a random environment[8] gives rise to clusters that look very much like DLA clusters.

Direct simulations of the DLA model makes very inefficient use of computer time. Several tricks have been developed to make DLA simulations tractable. One trick is that the random walker need not actually start far away from the aggregate. The walker can start at a random point on a circle of size R_{max} that just encloses the cluster because its probability of arrival on this circle is random. (This observation is due to M. E. Sander.) However, the walker may wander far away from the aggregate. In that case, it may take a long time for the walker to return to the smallest circle enclosing the cluster. This problem is not serious since it is possible to allow the walker to take large steps when it is outside R_{max}. To ensure that the walker does not encounter any matter, we allow the walker to take steps as large as the distance to the enclosing circle, but in a random direction. (This trick is due to P. Meakin.) A much more sophisticated way to do this is described below. In the most refined programs an additional trick is used: addressing techniques allow rapid location of the nearest point on the aggregate when the walker is inside a hole in a large aggregate. Then a step as large as the distance to this point can be taken, but in a random direction. Very large clusters can be grown very quickly this way.[10] For modest sizes that are necessary for the problems suggested here, this trick is not necessary.

Green's functions

An additional method used to grow large clusters is based on the physics of the situation, rather than additional

numerical techniques. A particle may walk outside R_{max} either on its first step or after wandering inside the circle for a while. It is likely to hit the boundary again near its current position. However, there is a chance that it will keep wandering outside R_{max} and hit again far away from its current position. Rather than taking computer time to let the particle walk around the outside the circle, we can instead find the probability density of the returning walker on the boundary and bring back the particle *in one jump.*

To compute this probability density, we define $u(\mathbf{r},t)$ as the probability that at time t a particle is at position $\mathbf{r}$, if at time $t=0$ the particle is at position $\mathbf{r}_0$. Note that $u(\mathbf{r},t)$ equals the probability of being at a neighboring position at the time of the previous walk. Thus if the grid points are at

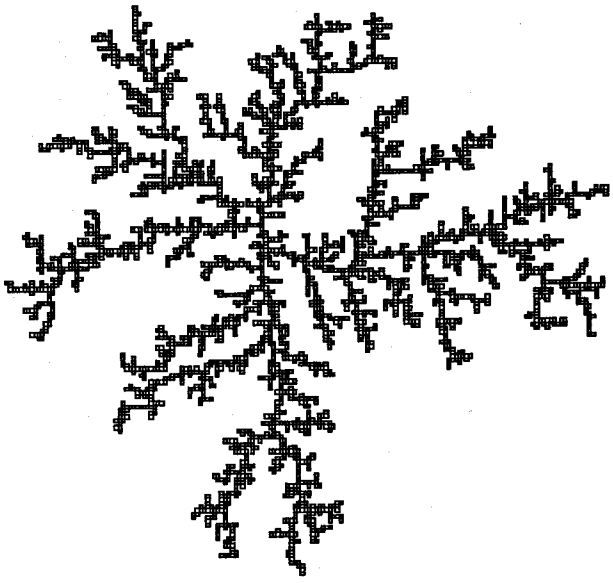

Figure 4. A (DLA) cluster of about 3000 particles. This cluster took ~10 min to grow on a Macintosh II. The program was written in True BASIC.

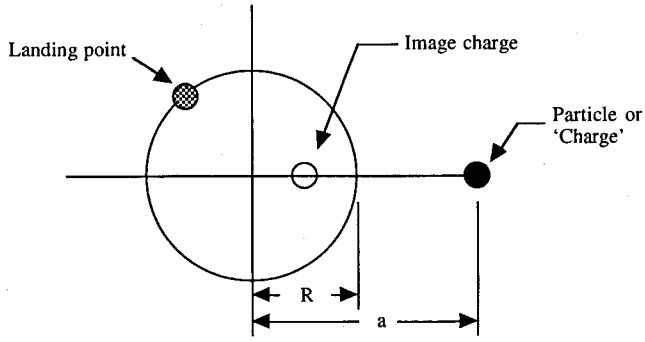

Figure 5. The geometry for working out the Green's function.

distance Δx from one another, and a walk occurs at intervals Δt, then the following relation holds in two dimensions:

$$u(x,y,t)=\tfrac{1}{4}[u(x+\Delta x,y,t-\Delta t)+u(x-\Delta x,y,t-\Delta t)+u(x,y+\Delta x,t-\Delta t)+u(x,y-\Delta x,t-\Delta t)]. \tag{3}$$

Equation (3) is the discrete version of the diffusion equation, $\partial u/\partial t=\nabla^2 u$, with initial condition $u(\mathbf{r},0)=\delta(\mathbf{r}-\mathbf{r}_0)$. We are interested in the total probability to land, which we call u_{tot}. If we integrate both sides of the diffusion equation from $t=0$ to ∞, we find

$$\nabla^2 u_{\text{tot}}=-\delta(\mathbf{r}-\mathbf{r}_0), \tag{4}$$

since $u(\mathbf{r},\infty)=0$. The solution to Eq. (4) is the *Green's function* for the Laplacian. Hence u can be thought of as the potential due to a point charge at $\mathbf{r}_0$ (a point charge in two dimensions or an infinite line charge in three dimensions). In our case $R_{\text{max}}=R$ is the radius of the circle containing the cluster, and $|\mathbf{r}|>R$. Because the circle is absorbing, we solve the equation under the boundary condition $u_{\text{tot}}=0$ on the boundary of the circle. This condition is equivalent to the electrostatic boundary-value problem of an infinite line charge parallel to an infinite conducting cylinder of radius R held at zero potential. Let $\mathbf{r}_0=(a,0)$ along the x axis for convenience (see Fig. 5). The solution to Eq. (4) is

$$u_{\text{tot}}\sim\ln\left(\frac{R}{a}\frac{|\mathbf{r}-\mathbf{r}_0|}{|\mathbf{r}-\mathbf{r}_1|}\right), \tag{5}$$

where $\mathbf{r}_1=(R^2/a,0)$. This solution can be obtained by using the method of images in two dimensions. You can check that $u_{\text{tot}}(R)=0$ by writing $|\mathbf{r}-\mathbf{r}_0|$ and $|\mathbf{r}-\mathbf{r}_1|$ in terms of the law of cosines.

The probability to land is the flux, the "electric field," through each point on the circle, $F=(\partial u_{\text{tot}}/\partial r)_R$. The integral of F from 0 to θ is the integrated probability ρ that the particle will hit the circle again before angle θ. We use Eq. (5) and normalize ρ and find

$$\rho=\frac{1}{2\pi}\int_0^\theta \frac{a^2-R^2}{a^2-2aR\cos\phi+R^2}\,d\phi$$

$$=\frac{1}{\pi}\tan^{-1}\left(\frac{a+R}{a-R}\tan\frac{\theta}{2}\right). \tag{6}$$

Note that $\rho=1/2$ at $\theta=\pm\pi$, i.e., there is a total probability 1/2 to wander all the way to the back of the circle either on the top or the bottom.

For our computer program we need to invert this function.[5] We choose a uniform random number between 0 and 1 and set it equal to ρ. Then we find the corresponding θ from Eq. (6) and put the particle at that point on the circle. It is easier to express this procedure in terms of the x and y coordinates of the landing point:

$$x=R\frac{1-\nu^2}{1+\nu^2},\quad y=R\frac{2\nu}{1+\nu^2},\quad \nu=\frac{a-R}{a+R}\tan\pi\rho. \tag{7}$$

If the initial particle is not on the x axis, we must rotate these formulas. If the initial position is $\mathbf{r}_0=(x_0,y_0)$ and $a=\sqrt{x_0^2+y_0^2}$, then

$$x=\frac{R}{a}\frac{(1-\nu^2)x_0-2\nu y_0}{1+\nu^2},\quad y=\frac{R}{a}\frac{(1-\nu^2)y_0+2\nu x_0}{1+\nu^2}. \tag{8}$$

If you use this method you should be able to generate fairly large DLA clusters with modest computing resources. There are many variations of the simple growth of a radial cluster with which you can experiment. You can consider growth in a channel, on a surface, with external fields, etc. These and many other variations have been tried in the literature, and many of them are very relevant to real experiments.

Our goal has been to introduce the field of random fractals and fractal correlations, one of the liveliest areas of statistical physics in the last decade. Many deep problems in the field are still unresolved. For example, there is no good understanding of why DLA makes fractal objects. As we have pointed out, practical applications of the models are numerous. The interested student can find much food for thought in the references.

Suggestions for further study

1. Show that by dividing the plane into triangular "boxes," the area covered by the Koch curve is zero. The area is bounded above by the total area of the triangles that cover the curve. You should find that, as the length of the triangles decreases by a factor of 3, the area of the triangles covering the curve decreases by a factor of 4/9. Hence as the length of the edge of the triangles goes to zero, show that the total area of the boxes that cover the curve goes to zero as well, and hence the curve has zero area.

2. Deduce the fractal dimension of the Koch curve using the results from Problem 1.

3. Implement the chaos game. Use the data points you find to show that the Sierpinski gasket has fractal dimension log 3/log 2. Use box counting for the calculation. Then look at the picture and find the dimension analytically.

4. Write a program that implements the algorithm in the text for spanning percolation clusters at p_c. Calculate the fractal dimension of the resulting objects. Use both box counting and correlation functions $R_g(N)$ and $C_t(N)$. Because this object is a statistical fractal, you need to average over many clusters. The average will be more or less the same whether you throw away or keep the nonspanning clusters. Here is an outline of the percolation algorithm:

(i) Start with a point (x_0,y_0) in the middle of your grid. Put this point on a list of populated sites.

(ii) Populate or block the neighbors of all the new sites on the list with probability p and $1-p$, respectively. Add the populated sites to the list. You should keep track of the number of newly populated sites. These new sites are at the same "chemical distance" from the starting point.

(iii) Repeat step ii until you either reach the edge of your grid, have added enough points, or until all sites are blocked.

When you find the dimension using $R_g(N)$, remember that at each N you need to sum over the distance from the center of mass $\mathbf{r}_0$. You can do this sum in a number of ways. One way is to use the following relation, which allows you to calculate R_g and related sums needed for calculating other quantities while you are computing points in the cluster:

$$\sum_{i=1}^{N} (\mathbf{r}_i-\mathbf{r}_0)^2=\sum_{i=1}^{N} \mathbf{r}_i^2-\frac{1}{N}\left(\sum_{i=1}^{N} \mathbf{r}_i\right)^2. \qquad (9)$$

For numerical reasons, it is bad to subtract two large numbers as is done in Eq. (9). To reduce the size of each term on the right-hand side of Eq. (9), try setting the origin of your grid such that $(x_0,y_0)=(0,0)$.

5. Write a program to implement the DLA algorithm and calculate the fractal dimension using box counting and correlation functions. Compare the answer you obtain using $R_g(\mathbf{x},r)$ with the one you find using $C_t(r)$. How did your answers compare in the case of the percolation model? Small DLA clusters do not seem to give the same answer for the two fractal dimensions, though the difference is small. This difference is probably due to the fact that the realizations are not homogeneous, because particles tend to stick at the outside of the cluster. It is possible that this difference goes away for large aggregates, though this point is still in dispute. It is not known whether DLA is a simple fractal or multifractal for which $D_0 \neq D_2$.

6. Modify your program for DLA so that it uses Green's functions; each time a particle walks outside the circle $R_{\max}$, choose a random number in the interval [0,1] and set it equal to ρ. From the discussion in the text you might be tempted to use the interval $[-1/2, 1/2]$. Why does this make no difference? The formulas (7) and (8) determine how far around the circle the particle is when it hits the boundary.

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