Chapter 8 Stochastic fractals; Self-reference in random phenomena

Goals

- To generalize our quantitative characterization of self-reference and dilation symmetry to random phenomena
- To gain an awareness of some well-known random phenomena with universal fractal properties
- To understand the Monte-Carlo method for simulating random phenomena.

8.1 Characterizing self-reference in random phenomena

The self-referential phenomena that we have seen up to now have been explicit, deterministic constructions. In this chapter we investigate how these qualities extend to random phenomena. Before proceeding, we recall the features of self reference that we have seen up to now.

The simplest form of self reference we encountered was that of the geometric series. Here the self-referential objects are mere numbers x_i. In this context the self-reference simply means that the relationship of x_{i+1} to x_i is the same as the relationship between the preceding pair of numbers x_i and x_{i-1}. The relationship in question is just the ratio of the two numbers. When the relationship is the same as one proceeds through the series, it means the ratio is constant and the series is geometric. The ratio is the defining quantitative means of characterizing the self-reference.

We next studied objects that were a step richer than simple numbers: sets of points in space, such as the Cantor set. Here too the points were organized in a series of pieces i. The ith piece has sub-pieces that are each the same as the whole ith piece. Each of the sub pieces is made of sub-sub-pieces the same way. Each piece defines itself by making reference to its sub-pieces. When a piece and a smaller sub-piece, and so on are the same. The object necessarily has a symmetry under transforming from the scale of the whole to the smaller scale of the sub-piece. In other words—a dilation symmetry. We saw that this symmetry could be aptly expressed using the methods of fractals. Here the quantitative characterization of self-reference was the fractal dimension D.

Next we encountered several self-referential qualities in iterative maps like the Logistic map. We found sequences of characteristic numbers—the fixed points x_i and the parameter values r_i marking analogous points in the period-doubling process. These points formed geometric series with its simple form of self reference. The function $g(z)$ resulting from many iterations of the initial function $f(x)$ was seen to have its own form of self reference embodied in the Feigenbaum equation. Moreover a new feature emerged: universality. The quantitative features of self reference that emerged from many iterations were independent of the independent of the starting point.

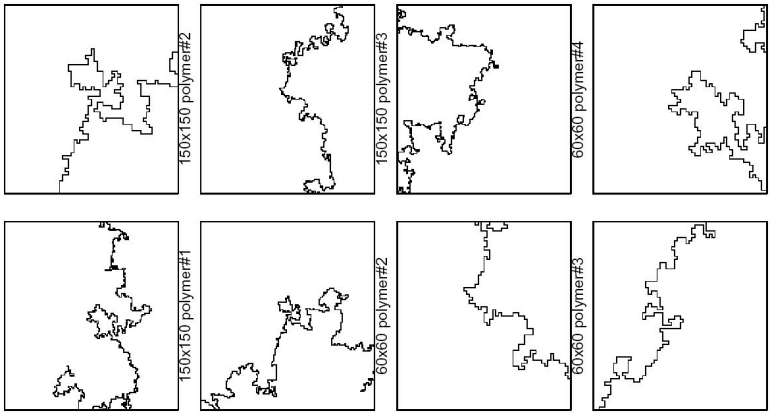

Figure 8.1 eight sections of a long self-avoiding walk, seen at two differing magnifications after Ref. 1.

All of these examples were made by deterministic, definite processes, with a definite starting point and an explicit prescription for each subsequent stage. In this chapter we turn to indeterminate processes in

which randomness plays an important role. Our main example will be the self-avoiding walk. To make such a walk, one begins with a point in the plane and then moves it randomly one unit up, down, left, or right. One repeats these moves many times for form an N-step random walk. One constructs an ensemble of all such walks. Finally, one examines each walk in the ensemble and discards it of the walk occupies the same point more than once. The remaining walks constitute the ensemble of self-avoiding walks. (Figure 8.1)

Our aim in this chapter is to look for the same kind of self-referential structure in such random objects as we formerly found in deterministic structures. Thus we are looking for the shapes seen in a section of a walk to be reproduced in subsections of that walk. Again, we are looking for some kind of invariance under *dilation*†. This is not the exact and identical invariance that we found in the Cantor set. Instead, we look for an invariance of the *ensemble* under dilation. One empirical criterion for this invariance is to imagine a sampling of many pictures of small pieces of a very long random walk and then a second set of pictures of this same walk but at a larger scale. Both sets of pictures have the same level of detail. We suppose that none of the pictures has enough resolution to see the individual steps of the walk. We give both sets to an observer and invite her to determine which set of pictures is the magnified set and which is the unmagnified set. If no statistical tests can distinguish one set from the other, then necessarily the ensemble is dilation-symmetric.

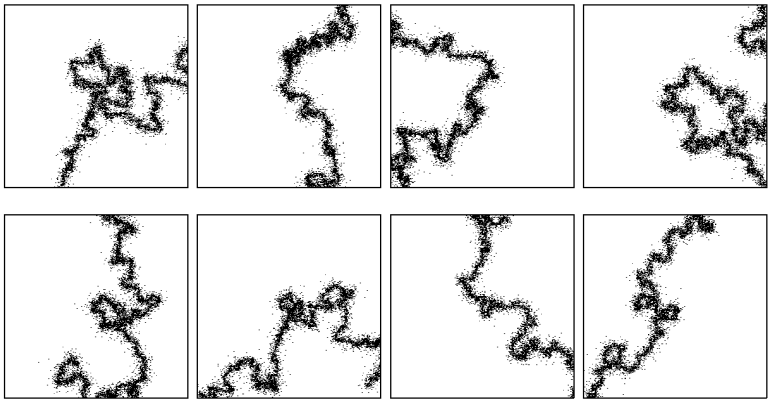

Figure 8.2 The walks pictured in Figure 8.1 at a low resolution such that the individual steps are not visible. After Ref. 1.

Using this logic we can come up with a quantitative measure of dilation symmetry. To do this, we think of the simplest statistical quantity measuring the spatial distribution of steps of the walk. This quantity is the density correlation function. The density $\rho(\vec{x})$ is defined for any point $\vec{x}$ in the space. (If we measure $\vec{x}$ in units of our basic step length, $\vec{x}$ must have integer co-ordinates.) It is defined for any particular walk in the ensemble: $\rho(\vec{x})$ is the number of steps of the walk that are at the point $\vec{x}$. For a self-avoiding walk $\rho(\vec{x})$ is evidently either 1 or 0 ‡. The simplest statistical average that provides spatial information about the walks is $\langle\rho(\vec{x})\rho(\vec{y})\rangle$. Here $\vec{x}$ and $\vec{y}$ are two different points and $\langle ...\rangle$ means "average over all members of the ensemble." Since we have not specified where we have placed our walk, this average cannot change if we move $\vec{x}$ and $\vec{y}$ by the same amount. It is convenient to choose the origin as y. It is also convenient to normalize $\langle\rho(\vec{x})\rho(0)\rangle$ by the average density $\langle\rho\rangle$. (Here no position variable is needed, since the average density cannot depend on position.) Evidently $\langle\rho\rangle$ is simply the probability that any given point is occupied. We denote the normalized quantity $\langle\rho(\vec{x})\rho(\vec{y})\rangle \,/\, \langle\rho\rangle$ as $\langle\rho(\vec{x})\rangle_0$; we call this the *local density at* $\vec{x}$. In words, $\langle\rho(\vec{x})\rangle_0$ is the average number of walk points at $\vec{x}$ given that the walk passes through the origin. Normalizing in this way assures that $\langle\rho(\vec{x})\rangle_0$ is independent of irrelevant features like how large a space we have placed our walks into.

† Dilation of a space normally connotes an expansion or magnification of the space. Here we shall use the word "dilation" to include either an expansion or contraction of the space, either a zoom-in or a zoom-out.

‡ We note that this ρ is defined at the scale of the elementary steps of the walk. The low-resolution pictures of Figure 8.2 also have densities ρ with similar dilation symmetry properties. However we need not consider these; the object itself has dilation symmetry over a range of magnification factors and distances $|\vec{x}|$ which are much larger than the elementary step size and much smaller than the object as a whole.

Remarkably the mere requirement of dilation invariance dictates the functional form of $\langle\rho(\vec{x})\rangle_0$. Dilation symmetry means that all statistical averages are essentially unchanged if one multiplies all spatial distances by an arbitrary factor λ. This makes sense in our system only if $\vec{x}$ is extremely large compared to the elementary step size. Then dilation symmetry means $\langle\rho(\lambda\vec{x})\rangle_0$ " = " $\langle\rho(\vec{x})\rangle_0$. The "=" means that we don't require strict equality in order to have the same spatial dependence of both sides on $\vec{x}$. It is sufficient if the two sides differ by some factor $f(\lambda)$ that does not depend on $\vec{x}$. Thus dilation symmetry implies

$$\langle\rho(\lambda\vec{x})\rangle_0 = f(\lambda)\,\langle\rho(\vec{x})\rangle_0\,. \tag{8.1}$$

As with the Cantor set, this dilation symmetry only becomes valid in the limit of a very long walk and with a restricted range of $\vec{x}$. Both $\vec{x}$ and $\lambda\vec{x}$ must be much larger than the step length and much smaller than the whole walk. For sufficiently long walks, the range of validity extends to as large a range of λ as we like.

We may readily deduce the form that $f(\lambda)$ must take. Evidently $f(1) = 1$, since a dilation with $\lambda = 1$ does nothing. Further, by making two dilations in sequence with scale factors λ_1 and λ_2, the result has to be equivalent to making a single dilation by a scale factor $\lambda_1\lambda_2$. Applying this fact to the law above yields $f(\lambda_1\lambda_2) = f(\lambda_1)f(\lambda_2)$. For any fixed λ_1 this fixes $f(\lambda_1\lambda_2)$ in terms of $f(\lambda_2)$. Thus it fixes the functional form of f. Evidently it is consistent with $f(\lambda) = \lambda^{-p}$, where p is an arbitrary power†

Knowing the form of f, it is now straightforward to determine the $\vec{x}$ dependence of $\langle\rho(\vec{x})\rangle_0$. First we note that all rotations of a given random walk are equally present in the ensemble, as are all translations. Thus $\langle\rho(\vec{x})\rangle_0$ cannot change if we simply rotate $\vec{x}$. It must depend only on $x \equiv |\vec{x}|$. We simply set $\lambda = 1/x$ ††. Then Eq. (8.1) implies

$$\langle\rho(\lambda x)\rangle_0 = \langle\rho(1)\rangle_0 = f(1/x)\,\langle\rho(x)\rangle_0 = (1/x)^{-p}\,\langle\rho(x)\rangle_0\,.$$

Thus $\langle\rho(x)\rangle_0 = x^{-p}(\langle\rho(1)\rangle_0)$: $\langle\rho(x)\rangle_0$ must be a power of x. Physically, the density of random-walk steps should fall off with distance. Thus the exponent p should be positive. We have determined much about the functional form of the density correlations given only the property of dilation symmetry.

This functional form is related to the fractal properties we have mentioned above. The fractal law for a set of points in space describes the number of points $N(R)$ within a distance R of a given point. Evidently in a statistical fractal this $N(R)$ depends on the chosen center point as well as the particular sample being studied. However, it is straightforward to relate the ensemble average of $N(R)$ to our normalized density $\langle\rho(x)\rangle_0$. Indeed, in two-dimensional space,

$$\langle N(R)\rangle = \int_{r<R} d^2r\,\langle\rho(r)\rangle_0\,.$$

Using the functional form of $\langle\rho(r)\rangle_0$, we deduce $\langle N(R)\rangle$ = constant R^{2-p}. Evidently if our object lived in three dimensions we would have $3 - p$ instead of $2 - p$, and similar in any dimension d We see that our dilation-symmetric objects in have a fractal property, with fractal dimension $D = d - p$. Our expectation that p should be positive amounts to the fractal dimension being smaller than the spatial dimension, as it is for all the fractal sets we have encountered.

This section has shown how the notions of self reference, dilation invariance and fractal dimension generalize naturally to statistical objects like self-avoiding walks.

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† To see this explicitly, we consider $df(\lambda_1\lambda_2)/d\lambda_2|_{\lambda_2=1}$. Using the chain rule, this derivative amounts to $\lambda_1 df/d\lambda|_{\lambda_1}$. On the other hand, using the law $f(\lambda_1\lambda_2) = f(\lambda_1)f(\lambda_2)$, this expression is evidently $f(\lambda_1)df/d\lambda|_{\lambda=1}$. Thus $\lambda f'/f = f'(1)$, which is independent of λ. This differential equation dictates the form $f(\lambda) = \lambda^{-p}$ for some constant p.

†† This λ, being smaller than 1, evidently represents a contraction, contrary to the conventional usage of "dilation", but in line with the contracted low-resolution images of Figure 8.2.

8.2 Universal statistical fractals

We discussed above how dilation symmetry in a random object like a self-avoiding walk leads to measurable properties, such as the exponents p and D. However, we never showed that self-avoiding walks are actually dilation symmetric. In fact they *are* dilation symmetric. This symmetry has been established by various mathematical and simulation approaches over the last three decades [2]. Moreover, the fractal dimension D is universal, just like the scale factors γ and δ in iterative maps. Here, universality means that one may make a wide range of variations in a self-avoiding walk, which may change its appearance markedly, without changing its fractal dimension D. In two dimensions self-avoiding walks have $D = 4/3$; in three dimensions $D \simeq 5/3$. For example, one may change the nature of the steps from mere nearest-neighbor steps to much more general random steps. One may also alter the rule of self-avoidance: any non-zero amount of self-repulsion turns out to be sufficient. We here briefly describe self-avoiding walks and other important statistical fractal phenomena. For more details on these phenomena see [3,2]

self-avoiding walks (Figure 8.2) The fractal properties of self-avoiding walks govern widespread physical phenomena. This is because the chainlike polymeric macromolecules that make up rubber, plastic, proteins, cellulose, and DNA behave statistically as self-repelling random walks [4]. For example, D enters into the law that predicts how the viscosity of a polymer solution grows with its concentration.

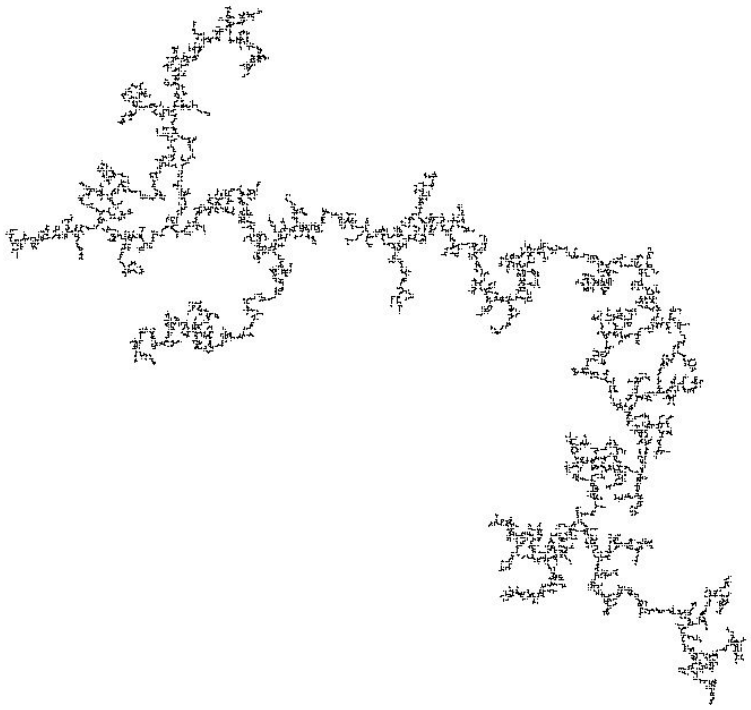

Figure 8.3 A 12000 particle lattice animal, after Ref 5.

lattice animals (Figure 8.3) If you place four stones on a Go board so as to make a connected cluster, there are only a few possible shapes. a straight line, a square, a knight's move, a zigzag. If you have a thousand stones instead of four, the number of possible shapes is large. These clusters are called lattice animals. The problem of characterising their shapes and enumerating them is challenging. It is also relevant for real-world phenomena, because certain macromolecules are synthesized by randomly assembling and disassembling such clusters. A powerful theorem [6] proved in the eighties shows that these clusters have a fractal dimension D of precisely 2 in three dimensions.

percolation Suppose that stones are placed at random, one by one on a very large Go board. Sometimes two stones will lie adjacent to each other, forming a connected cluster. As the number of stones increases, the likelihood of these dimers will increase, and larger clusters will appear. The size of the largest connected cluster grows steadily until at some point it spans the lattice. This point is called the percolation threshold. Several aspects of the shape of the large clusters are described by fractal properties. The most obvious is the cluster itself. Another is the convex outline or hull of the cluster. Percolation clusters are important in describing various types of propagation or contagion in a random medium.

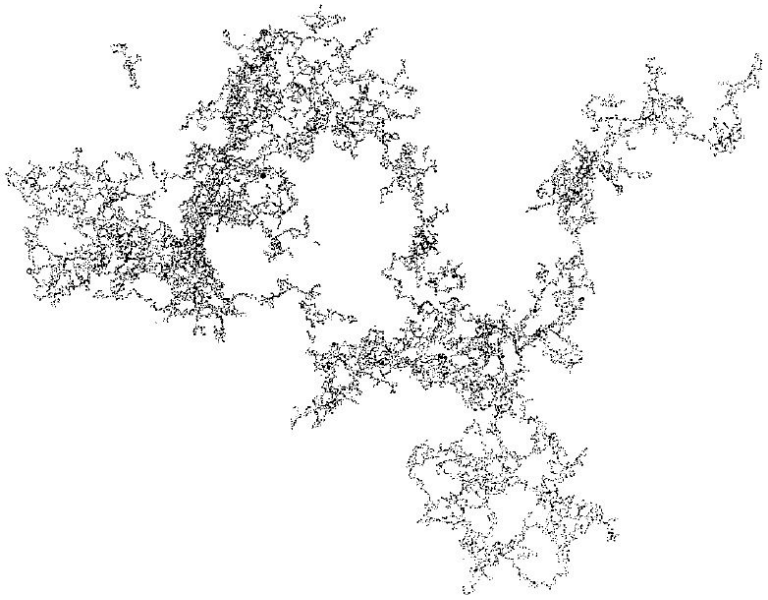

Figure 8.4 Electron micrograph of a diffusion-controlled colloidal aggregate of 5 nanometer colloidal silica particles, after Ref 1.

colloidal aggregates (Figure 8.4) Many large connected structures like carbon black or soot or composite snow flakes form when tiny bits of suspended solid matter are made mutually sticky so that they weld to each other on contact. As the suspended particles move and collide, they form dimers and larger clusters. Ultimately very large clusters can form. These clusters have been shown empirically to be fractals. There are several distinct fractal dimensions that can arise, depending on the growth process. The most common are diffusion-controlled clusters. Their fractal dimension is about 1.7 in three dimensions [7].

diffusion-limited aggregation (Figure 8.5) Place a single stone in the middle of a Go board. Then add a second stone far from the first one. Move it in a random walk. If it should happen to move adjacent to the initial stone, let it stay there. It becomes attached to the middle stone forming a cluster. Introduce a third stone at a large distance and make it walk like the second one did, until it visits a site next to the cluster. If one continues indefinitely in this way, ultimately a cluster of arbitrary size is formed. This is called a diffusion-limited aggregate or DLA. Diffusion-limited aggregates in two dimensions have a fractal dimension of about 1.7, like diffusion-controlled colloidal aggregates in three dimensions. Still DLA's are qualitatively different from diffusion-controlled colloidal aggregates. This model is a primitive example of diffusion-limited growth. It it thought to describe a wide range of growth processes where the addition of new material is limited by the rate at which material can diffuse to the growing object from far away. many mineral formations take this form.

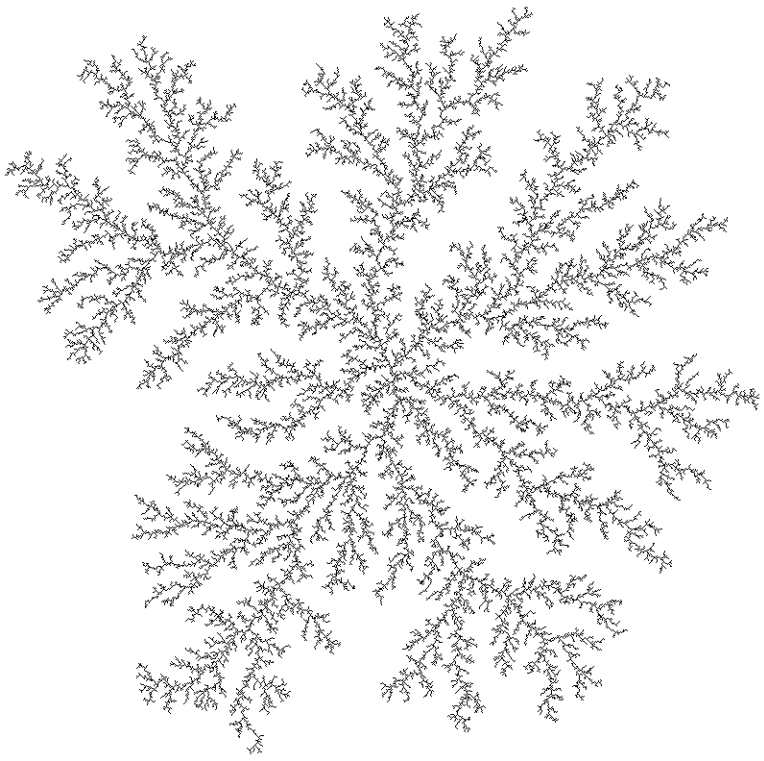

Figure 8.5 Simulated Diffusion-Limited aggregate after Ref 8.

8.3 Monte-Carlo sampling of random processes

The bulk of this course was devoted to the emergence of orderly self-referential scaling phenomena in deterministic dynamics. Similar orderly scaling occurs even when the underlying process is not deterministic but is intrinsically random, as noted in Chapter 1. In this section we briefly describe the most important method of exploring such random phenomena. It is called Monte Carlo sampling. We'll discuss the Monte Carlo strategy in the context of self-avoiding random walks.

When we wish to measure something about a random phenomenon, we are implicitly thinking about an *ensemble* of instances of that phenomenon. If the phenomenon is a self-avoiding random walk, we are interested in the ensemble of all possible such walks. To keep the counting simple, we'll consider walks on a square lattice starting from the origin whose first step is to the right. Then the ensemble of two-step walks contains three elements. The ensemble of three-step walks contains nine elements. The number of elements of N-step walks grows rapidly with N. We'd like to characterize these walks by measuring how average properties such as the end-to-end distance r vary with N. In order to find the ensemble average of, say r^2, we must add the (r^2)'s for each element of the ensemble and divide by the number of such elements. This is an impractical task, because there are so many elements.

We can gain information about the ensemble average by taking a random sample of s ensemble elements. Even though s is a small fraction of the total number of elements, its averages may be quite close to the true ensemble average. Of course, we want the choice of the s elements to be unbiassed; otherwise it can lead to incorrect averages.

Let's consider three methods of sampling the ensemble of self-avoiding walks.

a) Elimination This method consists of selecting an unrestricted N-step random walk at random and then discarding it if it intersects itself. Repeating this process sufficiently must lead to s self-avoiding walks. It is not difficult to select an unrestricted walk. One simply picks each of the N steps randomly from amongst the four possibilities. However, the discarding process proves deadly. Only an exponentially small fraction proves to be self-avoiding. Thus this elimination process is inefficient.

b) Growth Here we start with a one-step walk, and then add steps one by one, avoiding the previous steps

at every step. This growth process creates self-avoiding walks by construction. They are called kinetic self-avoiding walks. Sometimes the process gets stuck, because the last step is completely surrounded. Then one may remove a few steps and start growing again. This process generates self-avoiding walks much faster than the elimination process above. However, it is biassed.

To illustrate this bias, we consider a cousin of the self-avoiding walk. This is the ensemble of all connected clusters of sites, the lattice animals mentioned above. We simplify the counting by requiring that the origin be at the upper left. We may readily construct these objects by the growing method. For example, we may construct the cluster that forms a straight line to the right by sequentially adding particles to the right of the existing cluster, as shown in Figure 8.6

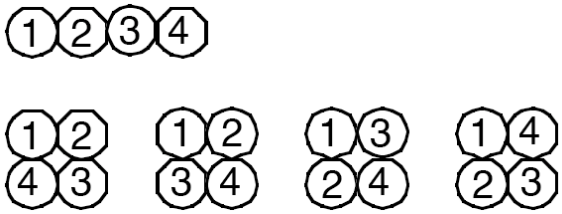

Figure 8.6 Two connected 4-site clusters sampled by growth. For each cluster, the set of growth sequences that can make it are shown.

From this picture it is clear that there are more ways to grow a compact cluster such as the square than for an extended cluster such as the line. Thus if clusters are grown at random, the square cluster will be sampled more often. The sampling is biassed. This famous case of bias has a major effect on the shapes. Unbiassed sampling in three dimensions leads to fractal clusters with fractal dimension $D = 2$. But the growth process leads to compact clusters with $D = 3$.

c) random changes of configuration Another possible strategy is to find one single element of the ensemble by some means or other, and then create other elements by modifying the starting element successively. If we can identify a type of modification that is capable of making every element of the ensemble and that doesn't introduce bias, such a strategy is a valid one. This is the Monte Carlo strategy.

unbiassed Monte-Carlo There is a general method of assuring unbiassed sampling in the Monte-Carlo strategy. To describe it, we label each element of our ensemble with the index c. Then the modifications or *moves* in our process consist of going from one element c to some other element c'. In order to sample the whole ensemble, these moves must be probabilistic. That is there must be a possibility of moving from a given c to a number of c's. Defining the Monte-Carlo process amounts to defining the probability of going from any given c to any given c'. We call the probability of going from c to c' $q(c'|c)$. It is a conditional probability of obtaining c' on the next step, given that the current configuration is c. The probability of going to *some* c' is evidently unity, so we must have $\sum_{c'} q(c'|c) = 1$. Now we imagine that we've done many of these moves to our initial configuration, so there is now a distibution of configurations. Suppose that the probability that the current configuration after i moves is c' is given by $p_i(c')$.

We can use q to find the new probabilities after one additional move:

$$p_{i+1}(c') = \sum_c p_i(c) q(c'|c).$$

We wish to find a rule that makes all the c's have *equal* probability after a long time. Thus as $i \to \infty$,

$$p_\infty(c') = \sum_c p_\infty(c) q(c'|c)$$

or, since all the p's are equal

$$1 = \sum_c q(c'|c). \tag{8.2}$$

This sum looks similar to the normalization sum $\sum_{c'} q(c'|c) = 1$. But it is not the same; the second argument is summed, not the first.

One way to assure that the condition of unbias is met, is to require that q obey the so-called *detailed balance* condition. This just means that the probability of a move is the same as the probability of the reverse move: $q(c'|c) = q(c|c')$, for all c and c'. Virtually all Monte Carlo simulations use q's that obey detailed balance. If q obeys detailed balance, then summing on either argument yields the same result: 1. Thus the condition of unbias is fulfilled.

There is a famous Monte-Carlo strategy to sample self-avoiding walks called the "slithering snake" algorithm. The process consists of many repetitions of the following steps:

i) Select an end of the current walk at random.
ii) Select one of the four lattice directions at random.
iii) Remove a step from the selected end and add it to the other end in the selected direction.
iv) Test whether this move creates an intersection. If it does, restore the original state.

By repeating this sequence, one can reach virtually any self avoiding walk from a generic initial state. Moreover, the process obeys detailed balance. To see this, consider a case where the attempted move is successful. To create this particular configuration c' from the current configuration c required a specific end and a specific direction to be chosen. The probability that the correct end was picked is 1/2; the probability that the correct direction was picked is 1/4. Thus the probability of reaching this c' from the original c is 1/2 * 1/4 = 1/8. Now we suppose that c' was the initial state. Again, a specific end and a specific direction must be chosen in order to reach c. The probability of this is evidently 1/8. Thus the direct and reverse moves have the same probability and our process obeys detailed balance.

The slithering snake algorithm has a deficiency. The detailed balance means that all *sampled* configurations are ultimately sampled with the same probability. But we have not yet shown that all self avoiding walks are in fact sampled. Indeed. there are self-avoiding walks that the slithering snake method can never find. For example, if both of the ends are completely surrounded by steps, it is impossible to add a step to either end. Thus all walks with blocked ends are inaccessible. There are many such walks, so this deficiency could potentially be important for some kinds of questions.

exercise An attractive alternative to the slithering snake alogorithm seems to be more efficient: In this alternative scheme, one performs steps i)–iii) as above, but in step iv), if an intersection occurs, one just tries a different bond direction. a) Exhibit allowed configurations c and c' where $q(c|c') \neq q(c'|c)$ in this scheme. b) Qualitatively, what kind of configurations do you think are favored by the resulting sampling bias?

8.4 Self-reference in thermal fluctuations

Concrete physical processes like phase transitions give rise to dilation-symmetric structures. Changes of phase such as the boiling of water occur because of thermal fluctuations. Normally phase transitions transform the matter into a greatly different state: *eg.* liquid water and water vapor. However, the degree of difference depends on the thermodynamic conditions like temperature. One may often identify a set of conditions at which this difference goes to zero. For water, this point is at a temperature of 642 Kelvin, and a pressure of 340 megapascal (about 30 atmospheres), where the density of both water and water vapor are about .320 times standard density [9]. Here liquid and vapor become indistinguishable. Then the water has no clear preference for one density or the other. It has strong fluctuations of density. It has been shown that these "critical" density fluctuations have scale invariance or dilation symmetry. The tools to show this involve finding a very simple realization of a phase transition. This simple realization, called the Ising model, plays the role of the logistic map in chaos theory.

Ising model A suitable simple model is the Ising model [2,3,10]. It describes a liquid-vapor transition using simplified configurations and simplified energies. In the Ising model the molecules are point particles that occupy the sites of a lattice; each site can be either occupied or empty. Now, molecules tend to make liquids because they attract each other. In the Ising model this attraction is represented by a potential energy u: every pair of adjacent particles contribute an energy $-u$. The total energy $E(c)$ is simply $-u$ times the number of adjacent pairs. As noted above, we see the critical fluctuations when we allow the liquid

to come to equilibrium at the right temperature and density. In the Ising model the proper density can be inferred by symmetry: it is 1/2: half the sites are occupied.

In order to simulate the Ising model, we must take account of the attractive energy and the temperature, absent in the self-avoiding chain ensemble. The energy and the temperature act by influencing the relative probabilities of the configurations c. Clearly if it is very cold, the system will ten to be in the lowest energy state. *i.e.,* it has as many adjacent pairs as possible. This makes a solid mass of adjacent particles with the rest of the lattice empty. Conversely if the system is very hot, the energy u is negligible, and thus the particles are placed at random in the lattice, irrespective of u. When a system is in thermal equilibrium, each configuration c has a particular probability $p(c)$ dictated by its energy $E(c)$ and the temperature T. For any pair of configurations c and c',

$$p(c')/p(c) = \exp(-E(c')/kT) \ / \ \exp(-E(c)/kT). \tag{8.3}$$

Here k is the famous Boltzmann constant discussed in all statistical mechanics text books. Evidently c's with low E(c) are more and more probable as T becomes lower.

biassed Monte-Carlo There is a straightforward way to make random changes in a configuration that give this thermal bias in $p(c)$. It is called the Metropolis algorithm and is discussed in Gould and Tobochnik [3]. It is a way of choosing the conditional probabilities $q(c'|c)$ of going from some initial configuration c to another one c'. Thus it is a generalization of our method for sampling random self-avoiding chains. We have seen that if $q(c|c') = q(c'|c)$ then $p(c') = p(c)$. this generalizes to biassed probabilities such that $p(c) = X(c', c)p(c')$. As above the Monte Carlo equation relating the $p_{i+1}(c)$ after the i'th step of the process to the $q(c'|c)$:

$$p_{i+1}(c') = \sum_c p_i(c) q(c'|c)$$

As above, we consider the probabilities $p(c)$ after many steps i such that $p(c)$ has become independent of i. If the resulting $p(c)$ have the desired bias $p(c) = X(c', c)p(c')$, then.

$$p(c') = \sum_c \left(X(c', c)p(c')\right) q(c'|c).$$

Dividing both sides by $p(c')$ we find $1 = \sum_c X(c', c)q(c'|c)$. Now if we choose $q(c'|c)$ such that $q(c|c') = X(c', c)q(c'|c)$ then $\sum_c X(c', c)q(c'|c) = \sum_c q(c|c')$†. The normalization condition on $q(c'|c)$ guarantees that this sum is 1, as required. Thus we have fulfilled the desired condition to make $p(c') = Xp(c)$.

To implement this scheme, we need only devise our Monte-Carlo moves to make our reverse moves X times as probable as the forward moves. Specifically $X(c, c') = e^{E(c)-E(c')/(kT)}$ Here is one way to achieve this [3]

i) Select a site at random in the initial configuration c;
ii) Exchange its contents with a random neighboring site to make a trial configuration c'. This exchange in general alters the number of adjacent particles near the two sites in question, so that it may change the energy E.
iii) If so, compute $X(c', c)$.
iv) If $X > 1$, adopt the trial configuration c'.
v) if $X < 1$ then adopt c' with probability X and revert to c otherwise.

Variants of this scheme are very widely used to simulate thermal fluctuations.

dilation symmetry Figure 8.7 shows two typical Ising configurations. The figure shows large, irregular areas growing as the temperature decreases. We may characterize these configurations as we did for the random walk, by choosing a black point and random and finding the average density of black for points at distance r. This density is precisely the quantity $\langle\rho(r)\rangle_0$ defined above. Here the dilation symmetry is slightly modified from that seen for self avoiding walks. The $\langle\rho(r)\rangle_0$ cannot vary simply as r to a negative power, since it must approach the average density—1/2—for large r. To see the dilation symmetry, we merely need to subtract this average density. One finds $\langle\rho(r)\rangle_0 - 1/2 =$ constant r^{-p}, where $p = 1/4$

† 28Nov2012. typo fixed: $\sum'$ replaced by $\sum$.

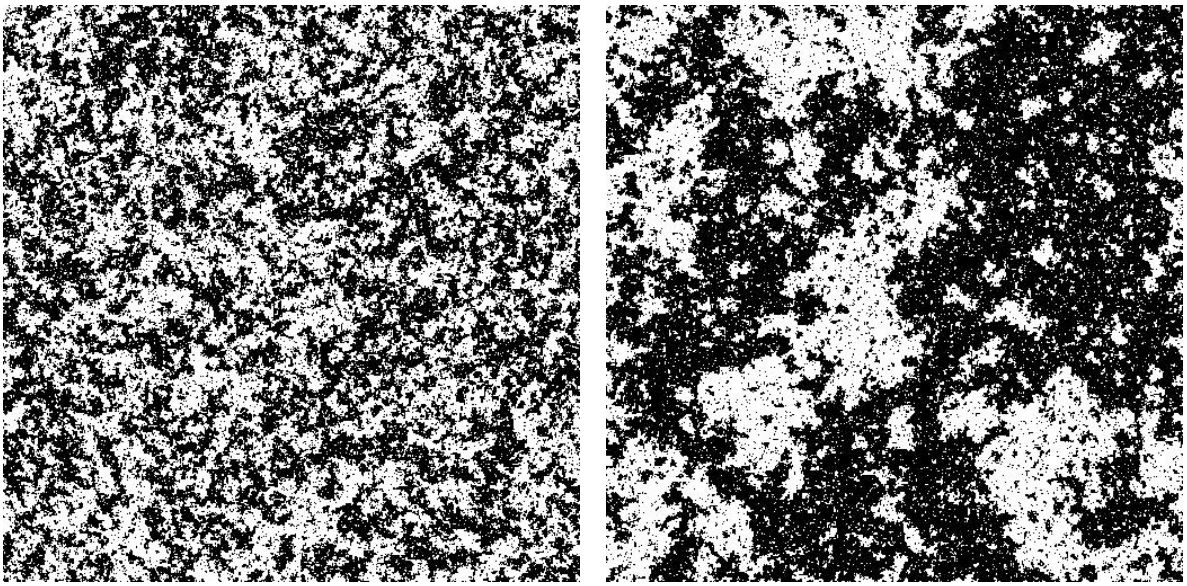

Figure 8.7 left: sampled Ising model configuration at a temperature ten percent above the critical temperature. right: at the critical temperature, after Ref 11.

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