CELLULAR AUTOMATA AND THE BOOTSTRAP PERCOLATION PROBLEM

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There are many problems in Physics that consider a particle that moves randomly through a medium. A question that arises is whether it is the particle or the medium to which the random nature can be assigned. In the former case, the problem is known as a diffusion process, and in the latter case it is a percolation process.

For example, consider the one dimensional Polya walk [Broadbent and Hammersley, 1957] in which a particle can move either left or right through a one-dimensional fluid. It can take steps of unit length to the left or right, each with probability of $\frac{1}{2}$. After an infinite number of steps have been taken, the particle would have visited an infinite number of points in the medium, each with probability 1. It is the particle which one can attribute the random nature, so this is a diffusion process.

Now consider it's converse. Suppose the medium itself is able to guide the particle left or right, each with a probability again of $\frac{1}{2}$. If the particle is guided in one direction, and then reaches fluid that tries to guide it in the opposite direction, it will become trapped. Here, after an infinite number of steps, only a finite number of points in the medium will be visited. It is the medium that has exhibits random nature, so this is a percolation process.

Percolation can be considered in free space, but it is most often considered in a regular, discrete medium, such as on a lattice or tree. Each vertex in the lattice is a *site*, and the connections between sites are *bonds*. It is the properties of the sites and bonds that determine the characteristics of the particular problem that is examined. For example, consider a network of pipes and valves. Each pipe is a bond, and each valve a site. Water can only flow through the network if there are pipes connecting valves and if the valves are open. If one considers a single valve, water can only flow into it if there is water flowing through a valve near it, and there is a pipe connecting the two valves. Thus, the effects upon a given site only depend on the sites and bonds near it.

Often, only bonds to the *nearest neighbors*, those sites of unit distance from the central site, are considered.

Some of the problems that can be solved with the percolation method are problems that involve spin systems. An Ising model considers sites as spins that have two states, an "up-spin" and a "down-spin." The energy of the configuration depends only on the orientation of nearest neighbor spins. Spins in opposite directions have a higher energy than spins in the same direction. Thus, the entire system can be assigned an energy that is dependent only on the local orientation of pairs of spins.

The pairs of spins that are considered depend on the type of lattice in the system. In the square lattice, for example, typically only bonds exist in the four cardinal compass directions, while on the triangular lattice, bonds can exist in any of six directions. The *coordination number* z of a lattice is the number of bonds permissible by the lattice, or, how many neighbors a given site can have.

One can also consider the two spin nature as being the presence or absence of an "atom" at a site - the site is either occupied or vacant. Typically, a probability is assigned in which a site is occupied (or vacant) with a probability p (or 1-p). *Clusters* of occupied sites then form because systems tend toward minimum energy. Clusters are groups of sites that are in the same state and adjacent to one another. Occupied sites are not in the same cluster if they are not adjacent to any site that is in the same cluster as the particular site.

Based on the value of p examined, different types of clusters form. A *critical concentration* p_c represents the point of a phase transition in the system. Below p_c, often many small clusters exist throughout the system. As p increases, these clusters grow and above p_c they have merged. On an infinite lattice, this cluster would contain an infinite number of occupied sites, so it is called the *infinite cluster*. Again, consider the pipe and valve network. If water enters a pipe at one end of the network, it cannot emerge at the other end unless there is a clear and open path across the network. The question can be viewed as "Consider a network of pipes and valves. How many valves on the average must I open in order for water to flow from one end of the network to the other?" i.e. "At what critical concentration does the phase transition occur?"

This is useful for explaining such systems as conduction bands in alloys. [Fuchs 1965] Adding more conducting atoms to the alloy does not make the alloy conductive until a certain concentration of these atoms has been reached.

Bootstrap percolation is a variation on the standard percolation model. Before the existence of an infinite cluster is tested, a *cull* is performed. Choose a neighborhood density m, $1 \leq m \leq z$, z the coordination number of the lattice. Examine the lattice and remove all sites that

have fewer than m neighbors. Repeat this procedure until no more changes can be made. (Note that all sites may become vacant as the cull is performed). Bootstrap percolation is useful for problems where a settling must occur. In magnets, for one, spins prefer to align in domains rather than independently throughout the material.

As you might expect, the addition of the cull can change the value of p_c for a given lattice. It can also be seen that for m=1, this problem reduces to ordinary percolation.

On trees, and in particular the Bethe lattice, it is possible to solve the bootstrap percolation problem exactly. On a Bethe lattice, it can be shown [Chalupa, Leath and Reich, 1979] that the transition is a first-order one. On a real lattice, however, the problem is more complex and the type of transition is unclear. It is not possible to solve the problem exactly for most lattices, but a numerical result can be obtained.

This problem lends itself well to cellular automata. Cellular automata consist of a lattice of cells where each cell can be in one of n states. A two-state cell is sufficient to model up-spins and down-spins, occupied or vacant sites. The evolution of a cell depends on the *rule* applied to it. Rules change the state of a cell often depending only on the states of nearby cells; the cells in its neighborhood. The application of a rule to all cells in the system occurs in a discrete time step. The new configuration is known as the next *generation* in the evolution of the automata.

For the bootstrap problem, rules were written to perform the cull and the spanning cluster mapping. An infinite cluster cannot exist on a finite lattice, so a cluster that spans across the lattice is taken as an approximation to the infinite cluster. The CAM-PC, a Cellular Automaton Machine for the IBM PC series of computers, was used to gather data. This machine can perform one generation on a grid of 256x256 cells in synchronization with an external 60Hz video monitor. Thus, sixty generations can be computed in one second, and the evolution of the system can be viewed in real time. Since all operations are done in hardware, this machine produces a much faster method of computing two-dimensional cellular automaton spaces when compared to more conventional methods, such as a program written in a high level language for a standard sequential machine, such as a UNIX workstation.

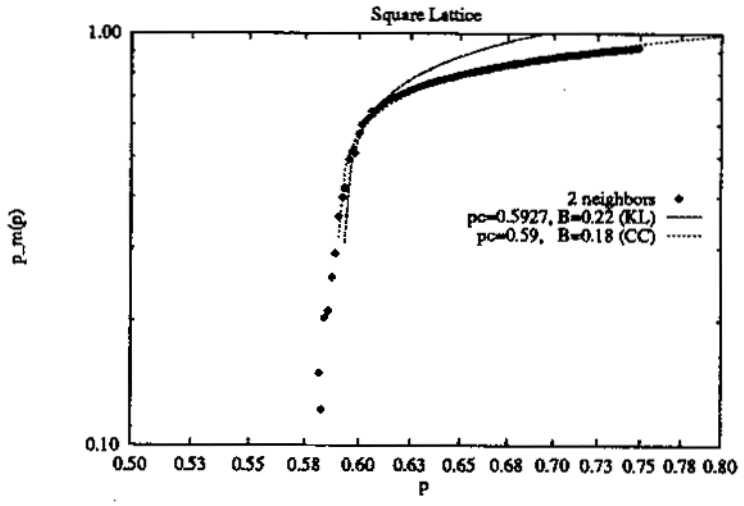
Software routines were written in FORTH, the language of the CAM-PC, and in C to generate, map, and analyze spanning clusters for several different neighborhoods and values of m.

When the cull is performed, the lattice is treated as if it has a periodic boundary. This allows the finite lattice to act as an approximation to an infinite lattice on which this problem would be ideally considered.

An aperiodic mapping is then performed. Occupied sites are made "active" on one side of the lattice, and a neighboring site becomes active in a succeeding generation if it contains an occupied site, and it is next to a site that has previously been made active. For this mapping, a boundary condition is imposed. The mapping is begun just within the border of the boundary, and the mapping is not allowed to continue through the boundary. This insures that the test for a spanning cluster is accurate. If at the end of the aperiodic mapping, some sites are active on the opposite side of the lattice from the start of the mapping, a spanning cluster must exist.

A periodic mapping is then performed. The aperiodic boundary is removed, and all sites are made inactive except for those sites that were on the far edge of the lattice from the start of the aperiodic mapping. These sites serve as the start of the periodic mapping. The size of this cluster, the spanning cluster, is then recorded. If the aperiodic mapping produced no active sites on the far edge of the lattice, the spanning cluster did not exist and its size is recorded as zero.

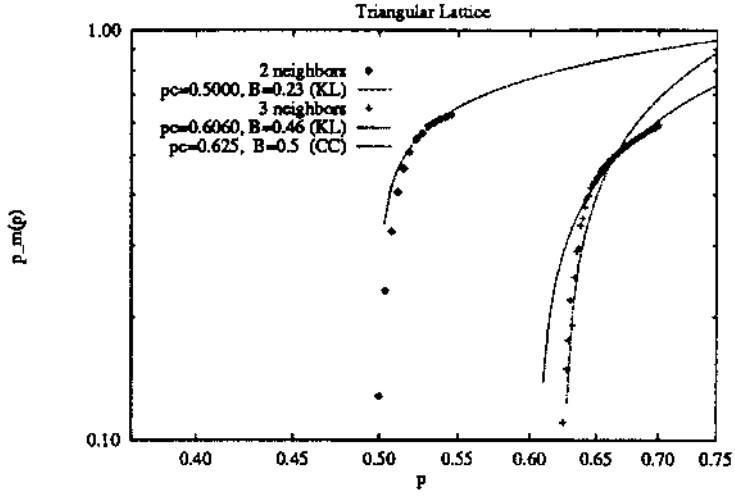
In the graphs that follow, the size of the spanning cluster is presented as a weighted average scaled to a percentage of the initial number of occupied sites. The weighted average reduces to the average size multiplied by a scaling factor. This scaling factor represents the probability of detecting a spanning cluster at that value of p.



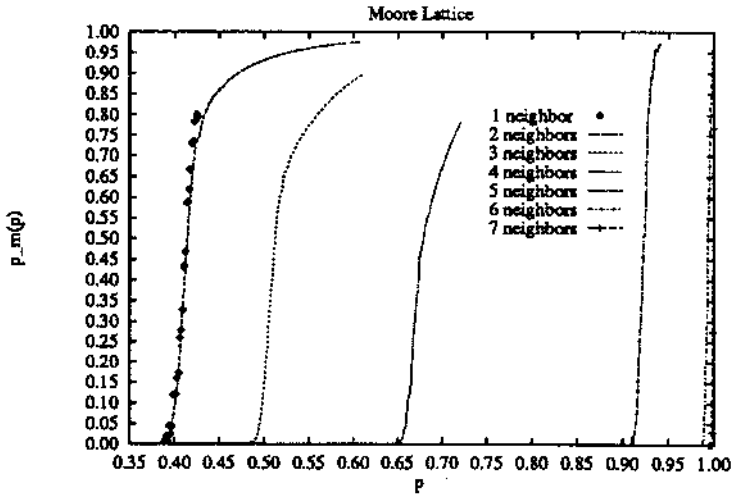
This log-log plot shows the square lattice for m=2. This curve exhibits a characteristic second-order phase transition. Theoretical curves of

$$A(p - p_c)^{\beta}$$

are superimposed. The curve as presented by Kogut (KL) [Kogut 1981] is plotted in addition to my own curve (CC). As can be seen, the critical parameters are similar.



This log-log plot shows the triangular lattice for m=2 and m=3. Again, both curves exhibit a second-order transition. For m=2, Kogut's curve fits well with this data. For m=3, however, there are differences. The most notable is the location of p_c. An estimate of p_c for my curve is about 0.02 higher, a significant difference. It was difficult to obtain a good curve fit though. A better value of p_c by inspection wouldn't allow a good value of β.



This plot shows the square lattice with the Moore (z=8) neighborhood. Curves for m=1 to m=4 seem typical of the transitions seen before. For m=5, the steepness of the transition may indicate something other than second order. For m=6 and m=7 however, the results are debatable. On a truly infinite lattice, m=7, and most likely m=6 as well, could not really exist. During the cull, an unstable vortex would appear and consume all of the occupied sites.

As you see, the CAM-PC is a useful piece of hardware for this problem, and can produce interesting results and a relatively short amount of time. The software written was able to produce data in accordance with previously published works, and may hint at something new for the triangular lattice with m=3 and the Moore lattice with m=5.

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