A fast algorithm for backbones

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A matching algorithm for the identification of backbones in percolation problems is introduced. Using this procedure, percolation backbones are studied in two- to five-dimensional systems containing $1.7 \times 10^7$ sites, two orders of magnitude larger than was previously possible using burning algorithms.

1. Introduction

In percolation models, the sites or bonds of a lattice are independently occupied with probability $p$, and the properties of the resulting clusters are studied. Above a critical density $p_c$, a cluster that spans the whole system exists, and one says that connectivity percolates. The backbone is defined as the subset of a connected cluster that carries current when a potential difference is applied between two points. The backbone of the spanning cluster determines the macroscopic transport properties of the system. At the critical concentration $p_c$, connected clusters and backbones are known to be fractals, although with different fractal dimensions. While geometrical properties of connected clusters have been numerically studied on very large systems containing as much as $10^{11}$ sites, backbone studies have been reduced to relatively small lattices due to the lack of efficient integer algorithms for backbone identification. The burning algorithm has been used by several authors, but this procedure is strongly CPU-limited and therefore it has not been possible to study systems of more than $2.5 \times 10^5$ sites.

Matching algorithms have been recently introduced for the related problem of rigidity percolation, and I show here that an extension of these methods can be applied to the study of connectivity percolation, allowing very efficient backbone identification for systems much larger than was previously possible using the burning algorithm.

2. The matching algorithm

Consider a system of $n$ sites $i = 1, \ldots, n$ connected by an arbitrary set $E$ of
Figure 1:  

- **a)** Before adding a new edge (ih) (dashed line) the following test is done:  
  - **b)** arrow (ki) is inverted, uncovering i.  
  - **c)** we uncover h by inverting the entire path (hgfe). Since both ends could be simultaneously uncovered, the new edge does not close a loop and therefore  
  - **d)** it is definitely added to D.

b bonds \( ij \) connecting sites \( i \) and \( j \). Bonds are initially labelled from 1 to \( b \), and sites are labelled from \( b + 1 \) to \( b + n \). The matching algorithm can be thought of as a clever way to identify and remove loops, and is implemented using a directed graph \( D \) as an auxiliary representation of the system. In this directed graph, lattice sites are represented by nodes \( i \) and bonds by directed edges \( ij \). We may think of each edge as an arrow. These can be pointing in either direction, subject to the constraint that no node has more than one arrow pointing to it. A node pointed to by an arrow will be said to be covered by the corresponding edge. A node with no incoming arrows is on the other hand uncovered. The directed graph \( D \) will be kept loopless. In order to do this, each time a closed loop (a cycle, or circuit) is identified (see later) it will be removed from \( D \), and replaced by a loop-node. A loop-node is a node in \( D \) that represents a deleted loop. Therefore, although initially there are as many nodes in \( D \) as there are sites in our system, as the algorithm proceeds we will delete some nodes and create loop-nodes. These loop-nodes will be given a loop-label, which is the minimum of all edge- and node-labels in the loop.

We start from a graph \( D \) initially containing \( n \) nodes and no edges, and add edges one at a time. Before adding an edge \( ab \in E \) to \( D \), the following test is done in order to know if a loop is closed by \( ab \): We attempt to reorganise the existing arrows (if any) on \( D \), in order to uncover both \( a \) and \( b \) simultaneously. Since by hypothesis \( D \) without edge \( ab \) has no loops, it must always be possible to uncover one of them. Let us then assume that \( a \) is uncovered first. If after doing this \( b \) can also be uncovered (while keeping \( a \) uncovered), then the new edge \( ab \) does not close a loop, and therefore it is definitively added to \( D \). This means: we add an arrow
We attempt to add a new edge (je) (dashed) to \( D \). First arrow (ij) is inverted, uncovering j. But now there is no way to uncover e while keeping j uncovered. This means that (ej) closes a loop. So now: start from e and follow arrows backwards, in this way identifying all edges and nodes in the loop (bold lines).

The loop is removed from \( D \) and replaced by a loop-node m. Between a and b, pointing to either of them (Fig. 2).

If on the other hand it is not possible to uncover b while keeping a uncovered (Fig. 2), this necessarily means that a loop would be formed on \( D \) by the addition of ab. In this case, edge ab is not added to \( D \) but the following is done instead: Starting from b (covered), we follow the arrows backwards. This will necessarily lead to a, thus identifying the new loop. All edges in this loop are given a common label \( l_{\text{min}} \), which is the minimum amongst all node- and edge-labels in the loop (including nodes a and b and edge ab). Next all nodes and edges in the loop are removed from \( D \) and replaced by a node with label \( l_{\text{min}} \).

There is an exception though, as eventually some of the nodes in this loop are connected to other nodes outside the loop (for example nodes i, f and g in Fig. 2). These are not removed from \( D \) but connected instead to the newly created node (node m in Fig. 2) by auxiliary arrows that initially point outwards. These auxiliary arrows have the same label as the loop-node. Also, some of the nodes that we do remove (nodes j, g and h in Fig. 2) may be eventually needed at later stages, for example if we have to add a new edge that connects to one of them. In such a case we simply recreate the corresponding node and connect it by means of an auxiliary arrow to the loop node.

The process of replacing identified loops by nodes is called condensation. It is possible to implement the matching algorithm without condensation. In this case, one simply does not add edges that close a loop but simply keeps track of the fact that a new loop has been formed by giving all loop-edges a common label.
Figure 3: A spanning cluster on a site-diluted square lattice of linear dimension $L = 64$ at the critical point. Bus bars are located on the left and right ends of the sample. Boundary conditions are periodic in the vertical direction. The removal of any critical bond (thick gray lines) would produce disconnection. In addition to those, ‘blobs’ of multiply connected bonds (thick black lines) also belong to the backbone. Dangling ends (thin lines) are connected to the backbone at one point only and are not relevant for macroscopic conductivity.

algorithm is perhaps simpler in this way. Condensation has on the other hand the effect of enormously improving speed and reducing memory requirements, since the graph size is decreased each time a loop is found. This is extremely important for large systems.

3. Backbone Identification

Imagine we want to know if two far apart points $a$ and $b$ on the system are connected, and in such case we want to identify the backbone $B(a, b)$ between these two points. This can be done by noticing that, if $a$ and $b$ are connected, then a long-range bond $ab$ would close a loop. Thus our method above serves to identify the parts of the system that belong to this loop, i.e. the backbone $B(a, b)$.

Therefore at any point we may simply do as if we were to connect a fictitious edge $ab$ between two arbitrary points $a$ and $b$ in the form described above, that is: we attempt to uncover both $a$ and $b$ on $D$. If this is possible, then $a$ and $b$ are not
connected. End. If only a but not b can be uncovered, starting from b follow the arrows backwards and in this way the backbone between a and b is identified. The visited edges are all critical, i.e. cutting one of the would produce disconnection of (a, b). These are called red bonds in the percolation literature. Some of the visited nodes will be loop-nodes. These are also included in the backbone, i.e. all edges that form the loops are, as well as all loop-nodes in them, in a recursive manner. Loop nodes are what is called blobs in the percolation literature. They are multiply connected so they contain no red bonds. If after identifying the backbone one is interested in also identifying the dangling ends, this can be done by ‘testing’ a fictitious bond between the backbone and all other nodes in the system. If a node is connected to the backbone then one cannot uncover both ends simultaneously. Thus the whole spanning cluster can be identified in this way (Fig. 3). But let us stress that dangling-end identification is not one of the strengths of the matching algorithm. This would be more efficiently done using for example a Hoshen-Kopelman type algorithm 2.

This is just a brief sketch of the main ideas about the matching algorithm. Several important issues have not been discussed in this paper, as for example how exactly nodes are uncovered in an efficient manner, data structures needed for computational speed, as well as a precise discussion of the relevant properties of the algorithm. A more detailed description will be published elsewhere 10.

4. Results

We present here partial results for scalar percolation on site-diluted hypercubic lattices in 2 to 5 dimensions. We start with a system containing no sites and add them one at a time at random locations. Each time a site is occupied, all new induced edges are tested and added to $D$ one at a time. Induced edges are those connecting the new site to already occupied nearest-neighbours. Loops are identified and removed as described in the previous sections. We proceed in this way until the percolation point is reached, which is detected because of the existence of a fictitious long-range bond connecting opposite sides of the sample. At this point, the density of occupied sites gives $p_c$ for this sample. We identify and measure the whole backbone (red bonds plus blobs) as well as the dangling ends at $p_c$ for each sample in this manner.

4.1. CPU time

Figure 4 shows CPU times per sample in seconds, needed to identify the whole backbone as well as the spanning cluster at $p_c$ versus linear sample size. Approximately half of that time is needed to identify the backbone alone, and the rest is used to obtain the dangling ends. Largest sizes simulated were $L = 4096$ in 2D, $L = 256$ in 3D, $L = 60$ in 4D and $L = 26$ in 5D. The number of samples varies between some thousands for the largest sizes to some millions for the smaller ones in each dimension. All runs were done on Alpha-500 workstations. Fits of the data
in Fig. 4 show that CPU-time scales with system size $n$ as $t \sim n^\theta$ with $\theta = 1.07$ (2D), 1.06 (3D), 1.05 (4D) and 1.05 (5D).

4.2. Correlation length exponent $\nu$

Since we add sites one at a time until the percolation point is reached, we are able to measure, for each sample, the critical density $p_c$ of occupied sites. The fluctuation $\sigma_L = \langle p_c^2 \rangle_L - \langle p_c \rangle_L^2$ of this quantity, were $\langle \rangle_L$ indicates averages over samples of size $L$, is expected to scale as $\sigma_L \sim L^{-1/\nu}$ with system size. Here $\nu$ is the correlation length exponent. On the other hand, rigorous arguments due to Coniglio show that the number $R_L$ of red bonds grows at $p_c$ as $L^{1/\nu}$.

Thus measuring $\sigma_L$ and $R_L$, two independent estimates for the thermal exponent $1/\nu$ are obtained. Figure 5 shows plots of $-\log(\sigma_L) / \log(L)$ and $\log(R_L) / \log(L)$ versus $1 / \log(L)$. We fit these data using

$$\frac{1}{\sigma_L}, R_l \sim L^{1/\nu} (1 + aL^{-\omega})$$

where $\omega$ is a corrections-to-scaling exponent. This allows the following estimates: $1/\nu = 0.75 \pm 0.01$ (2D), 1.13 $\pm$ 0.02 (3D), 1.44 $\pm$ 0.05 (4D) and 1.63 $\pm$ 0.05 (5D).

Correction to scaling exponents were found in most cases to be between 0.5 and
Figure 5: Fits of $-\log(\sigma_L)/\log(L)$ and $\log(R_L)/\log(L)$ versus $1/\log(L)$ for scalar percolation in 2 to 5 dimensions. The intercept at $1/\log(L) = 0$ is the estimated value of $1/\nu$.

0.8, but precise values cannot be given for these lattice sizes.

4.3. Backbone density at $p_c$

The fraction $B(L)$ of bonds on the backbone at $p_c$ is measured for several system sizes $L$ in each dimension. Our results are shown in Fig. 6.

Now assume $B(L)$ to behave as

$$B(L) = \lambda L^{-\beta'/\nu}(1 + aL^{-\omega})$$

where $d_b = d - \beta'/\nu$ is the backbone fractal dimension, and $\omega$ is an exponent of corrections to scaling. Fitting this expression with 4 free parameters to our data, we obtain the following estimates for the backbone fractal dimension: $d_b = 1.650 \pm 0.005$ (2D), $1.86 \pm 0.01$ (3D), $1.95 \pm 0.05$ (4D) and $2.00 \pm 0.05$ (5D).

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Figure 6: Backbone densities at $p_c$ for scalar percolation in 2 to 5 dimensions. Lines correspond to best fits using (2).

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