

The Diameter and Chemical Distance of Random Clusters

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Abstract

We report numerical results for the fractal dimension of the diameter (the “longest shortest path” between vertices along bonds) and the chemical distance of 2D and 3D Potts clusters for $q = 1, 2, 3, 4$. We find that the fractal dimension of the diameter and of the chemical distance of Potts clusters are equal within numerical error, and we suggest a possible relationship between D_{min} and the dynamical exponent, z .

The Potts Model, initially introduced as a generalization of the 2-state Ising Model to q possible spin states, can in fact be mapped onto the Random Cluster Model for all $q \geq 0$, with $q \rightarrow 1$ corresponding to the Percolation Model, and $q \rightarrow 2$ corresponding to the Ising Model. The Potts Model has found application in an impressively diverse range of contexts, including conformal field theory, percolation theory, knot theory, quantum groups, mathematical biology, and complex networks. Although easy to formulate, the model exhibits rich phase behavior, and its study has yielded many significant insights into critical phenomena in statistical physics.

An important geometric property of Potts clusters is the “chemical distance”, l – the length of the “chemical” or shortest path between two randomly chosen sites on a cluster. The average chemical distance on critical Potts clusters has been shown to scale as $\bar{l} \propto r^{d_{min}}$ at criticality, where r is the Euclidean distance between the endpoints of the chemical path l . Attempts to establish a relationship between d_{min} and other known critical exponents have as yet proved inconclusive. For the $q \rightarrow 1$ (Percolation) case, much work has already been done to determine d_{min} numerically [? ?] and an exact solution has been found using results from conformal field theory [?].

In this paper we generalize previous studies of d_{min} for the 2D, $q = 1$ Potts Model by reporting results for the $q = 2, 3$ and 4 for both Potts Models in both 2D and 3D. We also study the critical scaling of a related quantity: the diameter, D , defined as the longest of all the shortest paths between points on a cluster. We show that D also exhibits scaling behavior at criticality: $\bar{D} \propto r^{D_{min}}$; and that, significantly, $d_{min} = D_{min}$ to within the error in our numerical results.

We performed Monte Carlo simulations of critical q -state Potts model clusters in 2D and 3D using the Swendsen-Wang algorithm (SW) [? ?]. The q -state Potts model consists of a lattice of Potts spin variables σ_i , each of which can have integer values $\sigma_i = 1 \dots q$. Any two neighboring spins σ_i and σ_j contribute an amount $-K$ to the Hamiltonian if they have the same value, or zero otherwise; the Hamiltonian can thus be written as:

$$\mathcal{H} = -K \sum_{\langle i,j \rangle} \delta_{\sigma_i, \sigma_j}, \quad (1)$$

with K a dimensionless coupling constant.

The SW algorithm, which is itself based on the work of Fortuin and Kasteleyn [?], works by first introducing bonds between neighboring spins, with probability

$$p(\sigma_i, \sigma_j) = \delta_{\sigma_i, \sigma_j} (1 - e^{-K}), \quad (2)$$

thus creating clusters of bonded spins. All clusters thus formed are then, with probability $1/2$, “flipped” by choosing a random spin value from the q possible values, and assigning this value to all sites in the cluster. Such “cluster-flipping” algorithms dramatically reduce critical slowing down in computer simulations of spin models, as compared with algorithms that flip each spin individually [?] (e.g. the Metropolis algorithm [?]).

For each system of size L and given q at criticality, we first determined both the integrated autocorrelation time τ_{int} and the time to reach equilibrium τ_{equil} for the chemical distance l and diameter D of the largest cluster in each system. We then began the system with a random configuration and discarded the first 10^5 iterations (greater than $X\tau_{int}$) as a means of ensuring that each system reached equilibrium. We then ran each simulation for $10^5\tau_{equil}$. For some system sizes $L \geq 48$ we made several independent runs (using different random-number-generator seeds).

In order to illustrate our method for determining the chemical distance and the diameter of the clusters in our simulation, let us consider the special case of the Percolation Model (equivalent to the $q \rightarrow 1$ case of the Potts model) on the square lattice. In the Percolation Model, each edge or bond on the lattice is either “occupied” (with probability p) or “empty” (with probability $1 - p$). For $0 < p < 1$, finite-sized clusters of sites connected by bonds will form; at some critical value $p_c = 1/2$ there first appears, on average, a cluster that spans the lattice [?] (connecting, e.g., the top row of the square lattice to the bottom).

If we choose any two sites on such a cluster, A_1 and A_2 , the shortest path l along cluster bonds that connect the sites A_1 and A_2 is the “chemical path” [?] between these two sites. The diameter may then be defined as the longest of all such chemical paths on a cluster. These quantities are illustrated in Figure ??.

A typical method [refs] for determining l and d_{min} is the following. First, two sites A_1 and A_2 are chosen in the largest cluster in a particular realization of the system. Then a “Leath growth” process is begun at A_1 , and continued until A_2 is reached. The number of iterations in the Leath process corresponds to the l , the length of the chemical path between the two points. [[refs; discuss biases in this and in other methods in literature – e.g. bias towards smaller l Grassberger’s method]]. Then the Euclidean distance r between the two sites in the 2D or 3D grid is measured. After collecting many such measurements of l and r ,

one can then determine d_{min} by performing a three-parameter fit of the form $aL^b(1 + c/a)$.

Finding the diameter D exactly for a given cluster is equivalent to solving the all-pairs shortest paths problem for all possible pairs of sites in a given cluster; the computational complexity of the most naive solution scales as N^3 in the number of sites N . While many methods have been proposed [refs] for reducing the complexity of this task in the general case of undirected graphs to [[cite lowest figure in literature, with ref]], such algorithms are usually rather difficult to implement. Instead, we made use of the following two properties of 2D grid graphs: (a) the diameter of a graph embedded in a 2D lattice must have its endpoints on the perimeter of the graph; and (b) any “pins”, or singly-connected paths on the external perimeter of the cluster, contain vertices that can be eliminated as possible diameter endpoints; and it is straightforward to show that the existence of such a “pin” also allows us to eliminate candidate diameter vertices within the “body” of the cluster as well.

We thus need only consider a relatively small proportion [quantify this proportion, on average] of cluster sites as possible diameter endpoints, greatly reducing the number of “Leath scans” required in order to determine the diameter exactly.

Using these methods we were able to determine through numerical simulations the scaling exponents for the chemical distance d_{min} and for the diameter D_{min} for system sizes $L \times L$, $4 \leq L \leq 128$ in 2D and $4 \leq L \leq X$ in 3D. The results of these simulations (see Tables ?? and ??) indicate that d_{min} and D_{min} are equivalent to within error .

[Mean field limit?]