Bond-site percolation: empirical representation of critical probabilities

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LETTER TO THE EDITOR

Bond–site percolation: empirical representation of critical probabilities*

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Abstract. Our Monte Carlo simulations for mixed bond and site percolations on several 2D and 3D lattices show that the critical fractions p^{b*} and p^{s*} of bonds and sites follow the relationship $(\log p^{b*}/\log p_c^b)+(\log p^{s*}/\log p_c^s)=1$, where p_c^b and p_c^s are the critical fractions in the pure bond and site problems.

In mixed bond-site percolations connected structures are formed by contiguous arrangements of both bonds and sites or of either of these (Reynolds *et al* 1977, Heermann and Stauffer 1981, Zallen 1983). The model has been applied to polymer gelation (Stauffer *et al* 1982), to capillary phenomena in porous media (Yanuka 1989) and to fracture of porous concrete by cracks (Englman and Jaeger 1990). When one allows a fraction p^b of bonds and a fraction p^s of sites to exist in a lattice, the corresponding percolation probability function $P(p^b, p^s)$ will be zero for a pair of values $p^b < p^{b*}$, $p^s < p^{s*}$ and non-zero for values $p^b > p^{b*}$ and $p^s > p^{s*}$. The values $p^{b*}(p^s=1)=p_c^b$ and $p^{s*}(p^b=1)=p_c^s$ are well known (Essam 1972); however, for mixed percolation one has a family of values. For the latter, percolation will occur and an infinite cluster is formed at specific combinations of p^{b*} and p^{s*}.

An extensively studied situation is that where one requires in connected clusters that the sites are joined by (occupied) bonds and the bonds are joined by (occupied) sites (Agrawal *et al* 1979, De'Bell and Essam 1985). Both Monte Carlo simulations (Stauffer 1982, Yanuka 1989) and renormalisation group studies (Nakanishi and Reynolds 1979) yield p^{b*}–p^{s*} curves similar to those appearing in figure 1, which show our Monte Carlo results for a set of lattices in 2D and 3D, in which there is a single type of bond and a single type of site.

The results are well represented analytically by

$$p^{s*}=p_c^s(p^{b*})^{-\alpha} \tag{1}$$

where

$$\alpha=\log p_c^s/\log p_c^b. \tag{2}$$

Equations (1) and (2) can be rewritten as

$$\frac{\log p^{s*}}{\log p_c^s}+\frac{\log p^{b*}}{\log p_c^b}=1. \tag{3}$$

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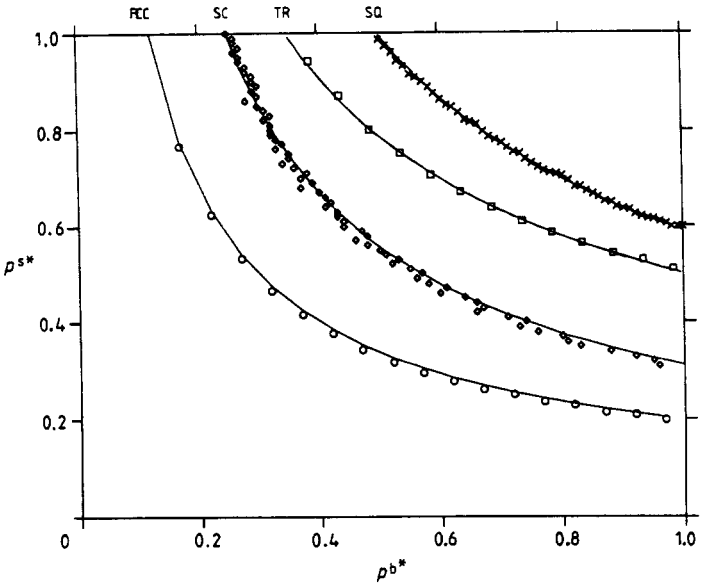

Figure 1. Critical mixed bond and site probabilities at percolation obtained by Monte Carlo simulations for the lattices: face-centred cubic (FCC), simple cubic (SC), triangular (TR) and square (SQ). The full curves follow (1) and (2).

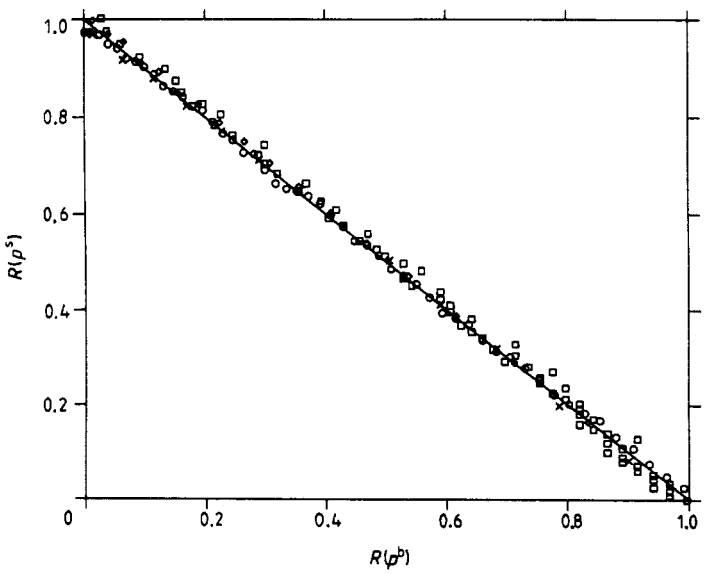

Figure 2. Representation of the data points in figure 1 according to (3) and (4), showing the fit to the diagonal (full line).

Using new variables

$$R(p^a)=\frac{\log p^{a*}}{\log p_c^a} \qquad (a=\text{s or b}) \tag{4}$$

the data of figure 1 collapse to a single line in accordance with (3) (figure 2).

To justify (3) we consider an artificial situation built upon a simple square lattice as shown in figure 3. We break up the original bond into several bond segments, designated b1, b2, ..., bi, ..., bn, whose fractional occupations are p^{b1}, $p^{b2}, \ldots, p^{bi}, \ldots, p^{bn}$ and also superimpose on each junction sites s1, s2, ..., sj, ..., sm whose occupations are p^{s1}, $p^{s2}, \ldots, p^{sj}, \ldots, p^{sm}$. We shall be interested only in the threshold, starred values of p and shall henceforth drop the stars for simplicity.

We seek a functional relation

$$F(p^{s1}, p^{s2}, \ldots, p^{sn}; p^{b1}, p^{b2}, \ldots, p^{bn})=1 \tag{5}$$

that has the following properties.

(1) F is a symmetric function of the bond probabilities and of the site probabilities.

(2) When two bond segments (say: bi, bj) are regarded as a single one (bk), so that its occupation probability follows the product rule, namely

$$p^{bk}=p^{bi}p^{bj} \tag{6}$$

the numerical value of F is unchanged and formally it contains p^{bk} instead of p^{bi} and p^{bj}. Similar considerations apply when two sites merge into a single one.

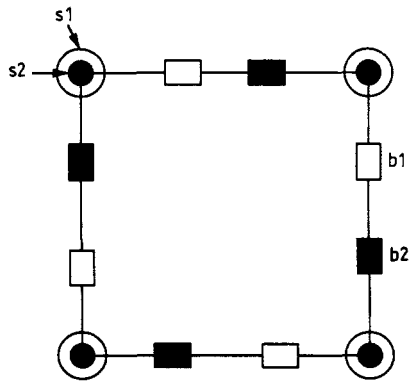

Figure 3. A cell of a square lattice containing multiple sites and bonds.

(3) When all variables except a single bond variable (say, p^{bi}), or a single site variable (p^{sj}) take their maximum value (=1) then a solution of (5) is

$$p^{bi}=p_c^{bi}$$

or, respectively,

$$p^{sj}=p_c^{sj}.$$

For the network in figure 3 all p_c^{bi} are equal (p_c^b, say) and so are all p_c^{sj} (=p_c^s).

The foregoing requirements strongly indicate the form

$$F(\{P^{bi}\},\{P^{sj}\})=\frac{1}{\log p_c^b}\sum_i \log p^{bi}+\frac{1}{\log p_c^s}\sum_j \log p^{sj}. \tag{7}$$

The two-term expression in (3) is a special case of this.

The mixed bond-site percolation network shown in figure 4 has two types of sites s1 and s2 and a single bond type b. The considerations that have led to the justifications of (3) suggest now the following equation:

$$\frac{\log p^{b}}{\log p_c^{b}}+\frac{\log p^{s1}}{\log p_c^{s1}}+\frac{\log p^{s2}}{\log p_c^{s2}}=1 \tag{8}$$

where by symmetry $p_c^{s1}=p_c^{s2}$.

We can attempt to find p_c^{s1} by considering (8) for the case when the sites s1 and s2 are equivalent. This means that the occupations of both site types are varied randomly in the same manner with the same mean occupations $p^{s1}=p^{s2}=p^{s}$.

The equation is

$$\frac{\log p^{b}}{\log p_c^{b}}+\frac{\log p^{s}}{\log p_c^{s}}=1 \tag{9}$$

in which the parameters are well known from the pure percolation problems, namely $p_c^{b}=0.5$, $p_c^{s}=0.593$. Comparing this with (8) for $p^{s1}=p^{s2}$ we find that $p_c^{b}=0.5$, $p_c^{s1}=p_c^{s2}=(0.593)^2=0.35$.

However, the latter value cannot be true for all varieties of the site occupations, since for $p^{s1}=1$ one has the value for critical concentration of the eight-coordinated site given by (Essam 1972)

$$p_c^{s2}(p^{b}=p^{s1}=1)=0.39.$$

The probabilistic explanation of the difference between the two values 0.35 and 0.39 is that, in the single-site percolation problem near the critical value 0.593, the realisations with about the same occupation fractions in the two types are more prone to be percolative than the realisations in which one site type is significantly more fully occupied than the other. This is why the $p^{s1}=1$ critical value for p^{s2} is higher than that for $p^{s2}\sim p^{s1}$.

In our computed results (8) is fairly well obeyed with $p_c^{s1}=p_c^{s2}=0.35$, except near $p^{s2}=1$, when the logarithmically plotted curves acquire a downward bend (figure 5). The plot of (8) with $p_c^{s1}=p_c^{s2}=0.39$ deviates from the diagonal. The difference in the

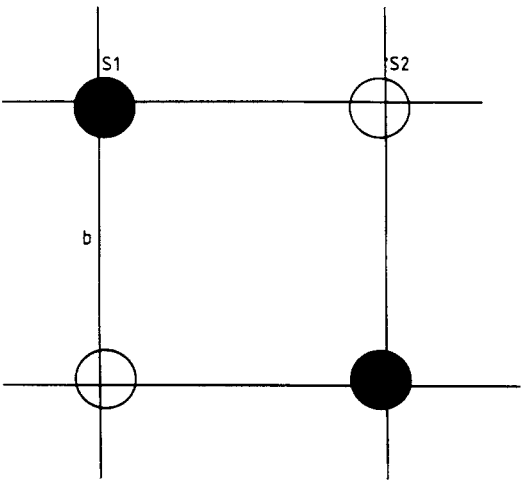

Figure 4. A square lattice consisting of two types of sites and a single type of bond.

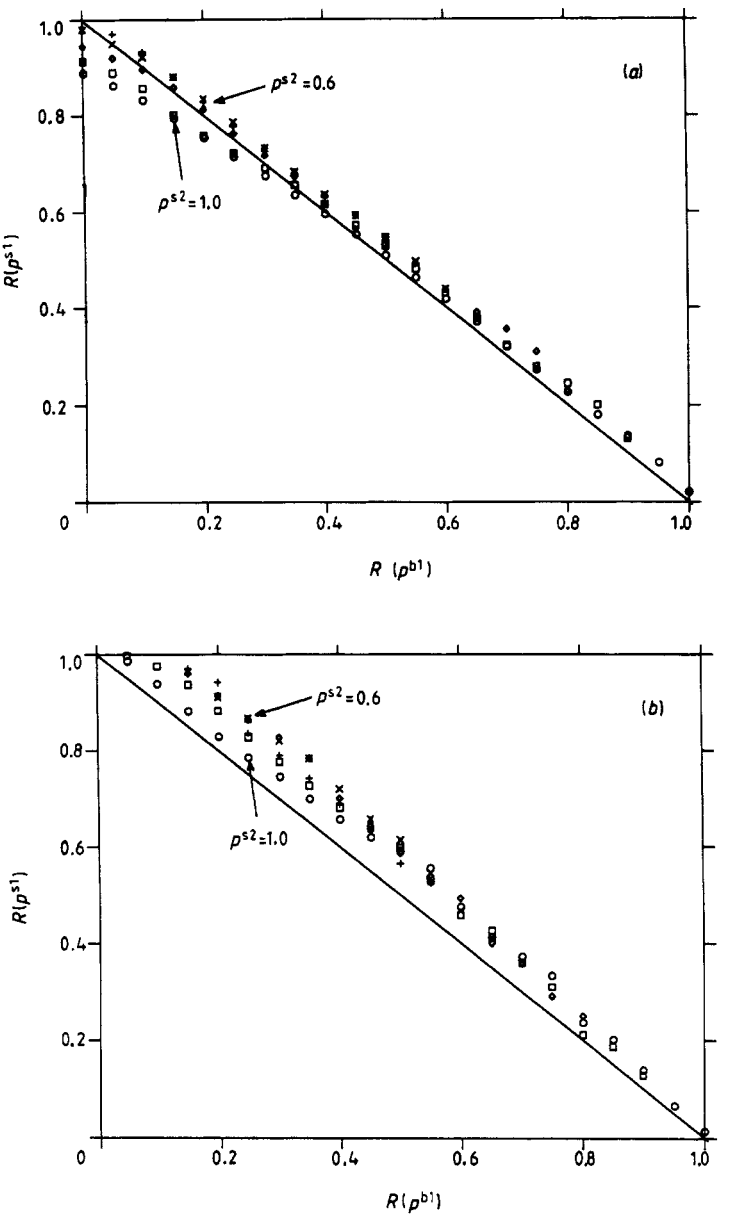

Figure 5. (*a*) Plot of Monte Carlo data for the lattice in figure 4 by use of the variables R in (4) for the following values of p_c^b: 0.6 (+), 0.7 (×), 0.8 (◇), 0.9 (□), 1 (○). The denominator of R has $p_c^b = 0.5$, $p_c^{s1} = p_c^{s2} = 0.35$. The straight line obeys (8). (*b*) Same as (*a*), but with $p_c^{s1} = p_c^{s2} = 0.39$.

two sets of plots attests to the sensitivity of the representation to even small differences in p_c^{s2} (=12%). Extensions of (3) and (7) are needed when the network contains parallel parts, namely those where one bond or junction can be severed (this is equivalent to putting their occupation numbers equal to zero) without precluding percolation by alternative pathways. In the simplest case one adds a second bond to the one already existing between neighbouring sites (figure 5). Then one can write out the equation

for the threshold values by replacing in (3) as follows:

$$p^{b*} \to p^{b1} + p^{b2} - p^{b1}p^{b2}. \tag{10}$$

For the parallel case the threshold occupations become reduced below their values in the absence of assistance from the alternative path. Then the ratio R in (4) exceeds unity (in contrast to the previous percolations, where $R \leqslant 1$) and it is natural to plot the solutions of (3) in a similar way to the reduced plot in figure 2 but having $R(p^{b1})^{-1}$ and $R(p^{b2})^{-1}$ as coordinates. Figure 7 shows several curves for various values of p_c^b (this is the threshold occupation for the combined bond connecting the sites when the site occupation is unity, $p^s = 1$).

Further work on the extension of the results described here will relate to more complex networks, requiring suitable topological classification, higher dimensions and continuum percolation.

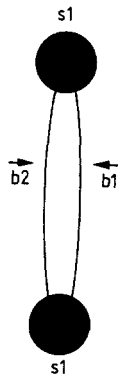

Figure 6. Two parallel bonds connecting sites.

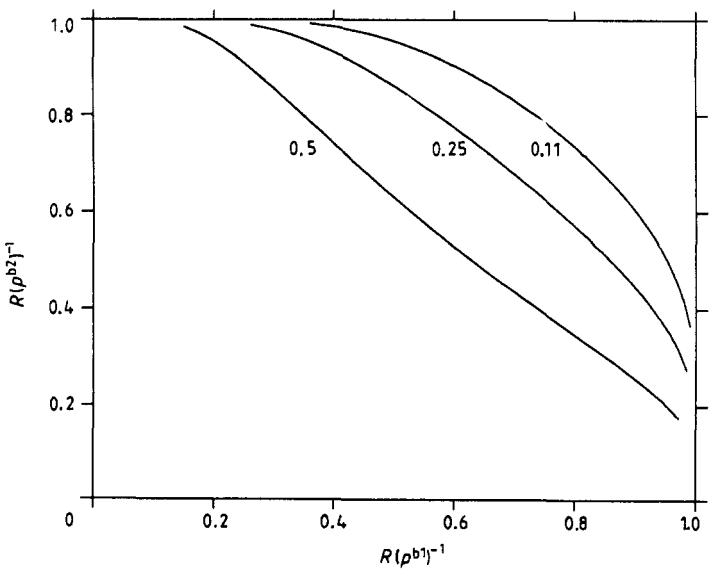

Figure 7. Plot of (3) in terms of the variables for the parallel bonds appearing in (10) using the inverses of the variables in (4) as coordinates. $p^s = 1$. Values of p_c^b are shown on the curves.

The solutions of (3) satisfy the following inequality, which can be derived from results proved by Hammersley (1980):

$$p_c^b < p^{s*} p^{b*} < p_c^s.$$

For a Bethe lattice (Zallen 1983) $p_c^b = p_c^s$, and the above inequalities collapse to the equation

$$p^{s*} p^{b*} = p_c^b$$

which is also the result of (3).

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