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Reciprocal relations for the weight factors arising in the series expansion of backbone percolation functions

R Brak†§, J W Essam‡ and M F Sykes†

† Department of Physics, King's College, Strand, London WC2R 2LS, UK
‡ Department of Mathematics, Royal Holloway and Bedford New College, Egham Hill, Egham, Surrey TW20 0EX, UK

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Abstract. We consider several properties of the 'backbone' of percolation clusters. The percolation model on a graph G is defined as follows. Each element (vertex or edge) of G is either 'open' or 'closed', the element e being open with probability p_e independently of all other elements. The u-v backbone in any configuration is the subgraph consisting of all elements which belong to at least one open, self-avoiding, path from a vertex u to a vertex v. We show that the expected value of any u-v backbone random variable Z, which depends only on the elements of the u-v backbone (e.g. Z may be the number of edges or the length of the shortest path of the backbone) is given by

$$E(Z) = \sum_{K \subseteq P} (-1)^{K+1} \tilde{Z}_K \prod_{e \in g(K)} p_e$$

where P is the set of all self-avoiding paths from u to v on G, $g(K)$ is the subgraph formed by all elements which belong to at least one self-avoiding path of K and the weight $\tilde{Z}_K$ is given by

$$\tilde{Z}_K = \sum_{J \subseteq K} (-1)^{J+1} Z_J$$

where Z_J is the value of Z when the backbone is $g(J)$. Certain 'reciprocal' relations are found to hold between the weights and the backbone variables in some important cases. Using these results, series expansions for the various properties can be obtained.

1. Introduction

We consider percolation on a graph G (or lattice L). We can define the percolation model on G as follows. Each element of G (vertex or edge) is considered either 'open' or 'closed', the element e being open with probability p_e independently of all other elements. A u-v path in a percolation model is a *self-avoiding* path (any path referred to below is assumed to be self-avoiding) between the two vertex elements u and v, and is said to be open if all its elements are open. The u-v backbone in any configuration is the subgraph consisting of all elements which belong to at least one open u-v path. The cluster C_u containing vertex u is the set of all elements which belong to some open path which starts at u. In physical applications it is useful to consider the passage of a 'fluid' which may, for example, be a liquid or an electric current from u to another vertex v. In such problems only the elements of C_u which form part of the u-v

§ Present address: Department of Theoretical Physics, Oxford University, 1 Keble Road, Oxford OX1 3NP, UK.

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backbone are relevant, since no flow can take place in the other elements, even though they are open.

Various statistics of the backbone (backbone variables) may be of interest depending on the application (Hong and Stanley 1983, Stanley 1977, Herrmann *et al* 1984, Coniglio 1982). We will consider nine properties of the backbone. The notation we will use for the various properties discussed below is summarised in the first row of table 1. The 'size' of the backbone may be measured by either vertex content, edge content or both, and will be denoted U since it is the number of elements of the chosen type in the union of all the open paths from u to v. Elements which lie on all open u-v paths are called nodal and the number of such elements (vertices, edges or both) will be denoted X since they lie on the intersection of the open u-v paths. Since u and v are always present in any union or intersection of u-v paths it is a matter of convention whether u and/or v are included in U and X. Nodal elements are critical in the sense that they would be the first to break down under excessive flow. We also consider the length $L^{\min}$ of the shortest u-v path which determines the time for the first arrival of fluid injected at u through to the vertex v.

Table 1. Reciprocal relations.

Property, Z:	U	X	$U^{\min}$	$U^{\max}$	$X^{\min}$	$X^{\max}$	$L^{\min}$	$L^{\max}$	γ
Weight, $\tilde{Z}$:	X	U	$X^{\max}$	$X^{\min}$	$U^{\max}$	$U^{\min}$	$L^{\max}$	$L^{\min}$	γ

We are principally concerned with the expected (or average) value of the backbone variables. Denote the value of a backbone variable by Z. It will be shown below that the expected value $E(Z)$ of the random variable Z is given by

$$E(Z)=\sum_{K\subseteq P}(-1)^{|K|+1}\tilde{Z}_K\prod_{e\in g(K)}p_e \tag{1}$$

where P is the set of all u-v paths on G, $g(K)$ is the subgraph formed by all elements which belong to at least one u-v path of K and the 'weight' $\tilde{Z}_K$, corresponding to the property Z, is given by

$$\tilde{Z}_K=\sum_{J\subseteq K}(-1)^{|J|+1}Z_J \tag{2}$$

where Z_J is the value of Z when the backbone is $g(J)$.

One of the main results of this paper is that all the terms (2^n if K contains n paths) in the sum of (2) reduce to a *single* term for the backbone properties we study. This results in a considerable reduction in effort when computing the weight, particularly for large graphs. We shall show that if $Z=U$ then $\tilde{U}_K=X_K$ in the sense that $\tilde{U}_K$ is the number of elements in the intersection of all paths of K. Thus, in place of evaluating Z_J for all the subsets $J\subseteq K$, it is only necessary to compute X_K for the single set K to obtain the weight. Similarly, if $Z=X$ then $\tilde{X}_K=U_K$. A similar 'reciprocal relation' exists between $L^{\min}$ defined as above and $L^{\max}$, the length of the longest open path from u to v.

The probability that v is connected to u is known as the pair-connectedness and is given by $E(\gamma)$, where $\gamma=1$ when there is at least one open path from u to v and zero otherwise. Clearly γ is a backbone random variable since it indicates the existence of a non-null backbone. We also show that γ is self-reciprocal, i.e. if $Z = \gamma$ then $\tilde{\gamma}_K = \gamma_K$.

The u-v 'elastic backbone' in any configuration is the graph obtained by taking the union of all elements in the set of shortest open u-v paths. These are the ones which would come under tension first, if u and v were pulled apart from one another. The size $U^{\min}$ of the elastic backbone is the number of elements in the above union. The number of nodal elements in the elastic backbone is denoted by $X^{\min}$. It is found that $U^{\min}$ and $X^{\min}$ are reciprocal to $X^{\max}$ and $U^{\max}$ respectively. The latter variables are the number of elements in the intersection and union of all longest open paths from u to v.

It is worth pointing out that our results apply to both directed and undirected graphs. In the directed case paths must respect the direction of the edges.

It is convenient for computational purposes (Essam 1972) to write the relation between $E(Z)$ and $\tilde{Z}_K$, given by (2), in the form

$$E(Z) = \sum_{g \in \Gamma_{uv}} W(g) \prod_{e \in g} p_e \tag{3}$$

where Γ_{uv} is the set of possible graphs which occur as u-v backbones and

$$W(g) = \sum_{K \subseteq P : g(K) = g} (-1)^{|K|+1} \tilde{Z}_K. \tag{4}$$

If $g(K) = g$, K is called a cover of g. Table 2 gives an example of how the weights $\tilde{Z}_K$, and hence $W(g)$, are calculated for several backbone properties. In table 2 the columns beneath each property contain the weights $\tilde{Z}_K$ for the corresponding sets of covering paths given in the left-most column. The sum of all the weights in a given

Table 2. Weight factors for the graph g whose random elements are the edges. The set P of u-v paths of g contains the paths A, B, C and D illustrated below. Only the covering subsets K of P are listed in the left-most column. The entries in the last row are the weights $W(g)$ and the remaining entries are the weights $\tilde{Z}_K$ corresponding to the property at the head of each column.

Covering subsets K	U	X	$U^{\min}$	$U^{\max}$	$X^{\min}$	$X^{\max}$	$L^{\min}$	$L^{\max}$
BC	−1	−7	−5	−3	−5	−3	−5	−3
ABC	0	7	5	1	5	5	5	3
ABD	0	7	0	0	7	7	3	3
BCD	0	7	5	1	5	5	5	3
ACD	0	7	5	0	5	6	5	3
ABCD	0	−7	−5	0	−5	−7	−5	−3
$W(g)$	−1	14	5	−1	12	13	8	6

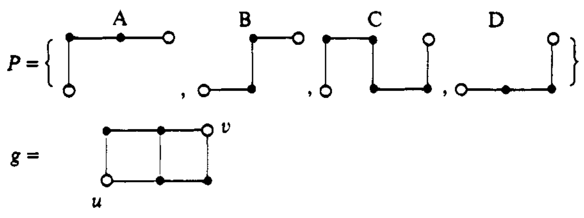
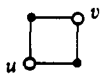
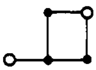
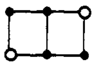
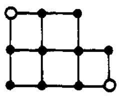


Table 3. Weight factors $W(g)$ of four graphs g, for the eight random variables considered. The random elements of the graphs are the edges and the open circles are the vertices u and v.

Graphs	Backbone variables							
	U	X	$U^{\min}$	$U^{\max}$	$X^{\min}$	$X^{\max}$	$L^{\min}$	$L^{\max}$
	0	−4	0	0	−4	−4	−2	−2
	−1	−5	−1	−1	−5	−5	−3	−3
	−1	14	5	−1	12	13	8	6
	17	−180	−70	65	—	—	−90	−72

column (as the subsets K of P are all covering) gives the corresponding weight $W(g)$ (shown at the bottom of each column). The weights $W(g)$ are given in table 3 for a selection of graphs.

For percolation on a crystal lattice L the sites of L are the vertices of G and the nearest-neighbour pairs (or bonds) are the edges. In site percolation $p_e = p$ or 1 depending on whether e is a site or bond and conversely for bond percolation. Interest centres on critical exponents which describe the behaviour of the expected values of the random variables when summed over v. These are calculated by analysis of the power series which result from (3). Generally the more graphs are included, the more accurate is the exponent. The nth term of these series may be computed by selecting all members of Γ_{uv} having n elements of the appropriate type.

2. General expression for $E(Z)$

Expected values in percolation theory are normally defined by considering the probability space in which the elementary events are the possible configurations of open and closed elements. Here we are considering random variables Z which in any configuration depend only on the elements of the u-v backbone. Since the u-v backbone is determined by the set of u-v paths which occur it is more convenient (although not strictly necessary) to consider a different probability space in which the sample points are the possible subsets of the set of all open u-v paths. In this space the expected value of Z can be written as

$$E(Z) = \sum_{J \subseteq P} \Pr\{J \text{ and only } J\} Z_J \tag{5}$$

where $\Pr\{J$ and only $J\}$ is the probability that the u-v paths contained in J, and only those paths, occur. It is convenient to express the probability in terms of the expected value of an indicator γ_i defined by

$$\gamma_i = \begin{cases} 1 & \text{if path } i \text{ is open} \\ 0 & \text{otherwise} \end{cases}$$

for then $E(\gamma_i) = \Pr\{\text{at least path } i \text{ is open}\}$ and hence

$$\Pr\{J \text{ and only } J\} = E\left(\prod_{i \in J} \gamma_i \prod_{j \in P \setminus J} (1-\gamma_j) \right)$$

where $P \setminus J$ is the complement of J with respect to the set P, thus

$$E(Z) = \sum_{J \subseteq P} Z_J E\left(\prod_{i \in J} \gamma_i \prod_{j \in P \setminus J} (1-\gamma_j) \right)$$

$$= \sum_{J \subseteq P} Z_J E\left(\prod_{i \in J} \gamma_i \sum_{J' \subseteq P \setminus J} (-1)^{|J'|} \prod_{j \in J'} \gamma_j \right).$$

Grouping together terms for which $J \cup J' = K$ gives

$$\begin{aligned} E(Z) &= \sum_{K \subseteq P} E\left(\prod_{i \in K} \gamma_i \right) \sum_{J \subseteq K} Z_J (-1)^{|K \setminus J|} \\ &= \sum_{K \subseteq P} (-1)^{|K|+1} \tilde{Z}_K \prod_{e \in g(K)} p_e \end{aligned} \tag{6}$$

where the weight $\tilde{Z}_K$ is given by

$$\tilde{Z}_K = \sum_{J \subseteq K} (-1)^{|J|+1} Z_J. \tag{7}$$

We note that for the empty set ϕ, $Z_\phi = 0$ and thus subsequently we shall only consider $\tilde{Z}_K$ with $K \neq \phi$.

Equations (6) and (7) are sufficient to obtain the expected value of Z on the graph G. The weights $\tilde{Z}_K$ depend only on the subgraph $g(K)$ and on the property Z. It will be shown in the following sections that (7) may be considerably simplified for each of the random variables of table 1.

3. Reciprocal relations

3.1. Union-intersection relation

Let X_J be the number of the chosen type of elements (vertices, edges or both) in the intersection of the paths J, and let U_J be the number of random elements in the union of the paths J. Then by the principle of inclusion and exclusion

$$U_K = \sum_{\phi \subset J \subseteq K} (-1)^{|J|+1} X_J \tag{8a}$$

which may be inverted to give

$$X_K = \sum_{\phi \subset J \subseteq K} (-1)^{|J|+1} U_J. \tag{8b}$$

If in (7) we set $Z = U$, the number of elements in the u-v backbone, then using (8b) gives

$$\tilde{U}_K = X_K \tag{9a}$$

similarly setting $Z = X$, the number of nodal elements, and using (8a) gives

$$\tilde{X}_K = U_K \tag{9b}$$

which establishes the reciprocal relation between U and X. It is also possible to obtain 'local' versions of (9) which refer to paths through a specific element e of the chosen type, as follows.

Consider the random variable U^e (or X^e) which indicates the event that e belongs to at least one (or all) open path(s) from u to v, then

$$U_K^e = \begin{cases} 1 & e \in \text{at least one path of } K \\ 0 & \text{otherwise} \end{cases} \tag{10a}$$

and

$$X_K^e = \begin{cases} 1 & e \in \text{all paths of } K \\ 0 & \text{otherwise.} \end{cases} \tag{10b}$$

We note that $E(U^e)$ is the probability that e is on at least one open path from u to v (i.e. belongs to the u–v backbone), and $E(X^e)$ is the probability that e lies on all open paths from u to v (i.e. is a nodal element of the u–v backbone). Clearly

$$U_K = \sum_e U_K^e \qquad X_K = \sum_e X_K^e.$$

Equations (8) are summed forms of the formulae

$$U_K^e = \sum_{\phi \subset J \subseteq K} (-1)^{|J|+1} X_J^e \tag{11a}$$

$$X_K^e = \sum_{\phi \subset J \subseteq K} (-1)^{|J|+1} U_J^e \tag{11b}$$

which occur in standard derivations (Chung 1974) of the principle of inclusion and exclusion. Setting $Z = U^e$ in (7) and using (11b), we obtain

$$\tilde{U}_K^e = X_K^e$$

and similarly with $Z = U^e$ we find, using (11a)

$$\tilde{X}_K^e = U_K^e$$

which are the analogues of (9). We note that

$$\tilde{U}_K = \sum_e \tilde{U}_K^e \tag{12a}$$

$$\tilde{X}_K = \sum_e \tilde{X}_K^e. \tag{12b}$$

When $E(Z)$ is calculated by a computer it is far more economical to calculate $\tilde{Z}_K^e$ for each element (and then use (12)) since in (5) it is possible to replace P by P^e, the set of paths from u to v which contain e. This considerably reduces the number of subsets which need be considered in (4).

3.2. Longest–shortest relation

We first consider variables Z_J which depend only on the shortest paths in J. The variable and its weight will be labelled by a superscript min. Let $K_{\max}$ be the subset of paths of K of *maximum* length, and let $K_{\min}$ be the subset of paths of K of minimum length, then from (7)

$$\tilde{Z}_K^{\min} = \sum_{\phi \subset J \subseteq K_{\max}} (-1)^{|J|+1} Z_J^{\min} + \sum_{\phi \subset J' \subseteq K \setminus K_{\max}} \sum_{J'' \subseteq K_{\max}} (-1)^{|J'|+|J''|+1} Z_{J' \cup J''}^{\min} \tag{13}$$

where we have used $Z_\phi = 0$. Since $Z_{J' \cup J''} = Z_{J'}$, (13) can be written as

$$\tilde{Z}_K^{\min} = \sum_{\phi \subset J \subseteq K_{\max}} (-1)^{|J|+1} Z_J^{\min} + \sum_{\phi \subset J' \subseteq K \setminus K_{\max}} (-1)^{|J'|+1} Z_{J'}^{\min} \sum_{J'' \subseteq K_{\max}} (-1)^{|J''|}$$

and using

$$\sum_{J \subseteq K_{\max}} (-1)^{|J|} \equiv 0 \tag{14}$$

one obtains

$$\tilde{Z}_K^{\min} = \sum_{\phi \subset J \subseteq K_{\max}} (-1)^{|J|+1} Z_J^{\min}. \tag{15a}$$

Thus a variable whose value depends only on the shortest paths has a weight which depends only on the longest paths in K. Similarly if $K_{\max}$ is replaced in (13) and (14) by $K_{\min}$ then if Z only depends on the longest paths (denoted with superscript max) equation (15a) becomes

$$\tilde{Z}_K^{\max} = \sum_{\phi \subset J \subseteq K_{\min}} (-1)^{|J|+1} Z_J^{\max}. \tag{15b}$$

Thus if Z_J depends only on the longest paths in J, it has a weight which depends only on the shortest paths in K. These are the longest-shortest reciprocal relations. The remaining reciprocal relations referred to in the introduction are special cases of (15). We conclude by considering each of these in detail.

3.2.1. Union-intersection relation for shortest paths. Now consider $U^{\min}$ (or $U^{\max}$), the number of elements in the union of the shortest (or longest) paths, and $X^{\min}$ (or $X^{\max}$) the number of elements in the corresponding path intersections. Then from (15a)

$$\tilde{U}_K^{\min} = \sum_{\phi \subset J \subseteq K_{\max}} (-1)^{|J|+1} U_J^{\min}$$

and using (8b) gives

$$\tilde{U}_K^{\min} = X_K^{\max}.$$

Similarly with $Z = X^{\max}$ in (15b), and using (8a), gives

$$\tilde{X}_K^{\min} = U_K^{\max}.$$

We note that $U^{\min}$ and $X^{\min}$ are the size and number of nodal elements of the u–v elastic backbone.

3.2.2. Union-intersection relation for longest paths. Similarly to §3.2.1, but with $Z = U^{\max}$, one obtains by using (15b)

$$\tilde{U}_K^{\max} = X_K^{\min}$$

and with $Z = X^{\max}$ one obtains

$$\tilde{X}_K^{\max} = U_K^{\min}.$$

3.2.3. Longest-shortest lengths relation. Finally we consider $L^{\min}$ (or $L^{\max}$), the length of the shortest (or longest) path from u to v. Then from (15a)

$$\tilde{L}_K^{\min} = \sum_{\phi \subset J \subseteq K_{\max}} (-1)^{|J|+1} L_J^{\min} = L_K^{\max}$$

since the length of the shortest path in any subset of $K_{\max}$ is always the length of the longest path in K. Thus the shortest length weight for subset K is just the length of the longest path in K. Similarly if $Z = L^{\max}$, then from (15b) one obtains

$$\tilde{L}_K^{\max} = L_K^{\min}.$$

3.2.4. Pair-connectedness self-reciprocal relation. The pair-connectedness indicator γ is self-reciprocal in the sense that if $Z = \gamma$ then $\tilde{\gamma}_K = \gamma_K$. This can be seen by substituting γ into (7) and using (14) with $K_{\max}$ replaced by K.

All the above reciprocal relations between the property Z and its weight $\tilde{Z}$ are summarised in table 1.

4. Conclusion

We have considered several backbone percolation properties and derived general expressions (equations (3), (4) and (7)) which can be used to calculate the expectation value of a backbone property. The calculation reduces to evaluating the weights of a set of graphs. Of principle importance has been the simplification of the expressions used to compute the weights, equation (7). We have shown that the weight expression reduces to a single term for all the properties considered and that reciprocal relations exist between the weights and the properties. When the property depends on the union of paths its weight depends on the intersection of the paths and conversely, if the property depends on the intersection of the paths its weight depends on the union of the paths. This is the union-intersection reciprocal relation. Similarly, if the property depends on the length of the longest paths then its weight depends on the length of the shortest paths (and vice versa). This is the longest-shortest reciprocal relation.

The simplication of the weight expression considerably reduces the amount of computation required to evaluate the weights. The above results have been used to derive series expansions for each of the properties (Brak 1986). An analysis of the series then enables critical exponents to be obtained. As the accuracy of the exponents generally depends on the length of the series, any method which enables the series to be extended is of considerable value.

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