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Percolation Pattern in Continuous Media and Its Topology

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Abstract. Continuum percolation problem is formulated with use of a random Gaussian field. Topological considerations are applicable to this continuum model. The specific Euler characteristic (EC) is calculated for any dimension d which is to be extended to a continuous variable by an analytic continuation. It is used to compose a phase diagram characterizing the connectivity of percolation patterns.

What is concerned with in the percolation problem is the spatial connectivity of random stochastic patterns. One of the most simplified example which is called a site problem is shown in Fig. 1. Each site on an infinitely extended lattice is independently occupied by a particle with uniform occupation probability p. Define a pair of neighbouring sites to be connected if both sites are occupied, then one may obtain various types of randomly connected clusters. When the probability p is increased, an infinitely connected cluster would be found. This is called a percolating cluster. An alternative way to define such random clusters is a bond problem shown in Fig. 2. Here each line between a pair of neighbouring sites is independently occupied by a bond with probability p.

Interesting problems in the percolation theory are classified as follows:

1) What is the critical value of p for percolation? The critical value p_c is defined as the occupation probability p above which the probability for a pair of infinitely distanced sites to be connected in a cluster is finite. The explicit value p_c depends on the lattice type including its dimensionality and the definition of the problem quoted above.

2) Is the percolating cluster at p_c a fractal object? The critical cluster makes a statistically self-similar pattern, i.e., a typical example of fractal graphs. (Takayasu,

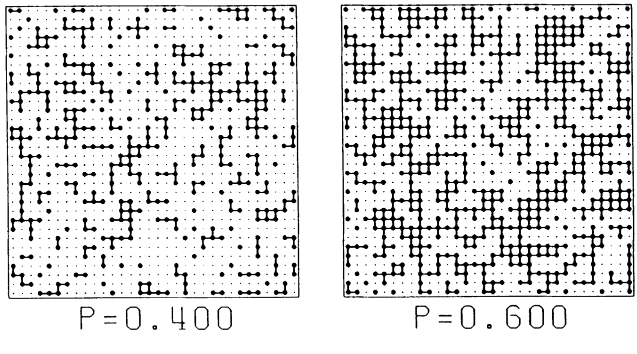

Fig. 1. Nearest neighbor site problem on a square lattice.

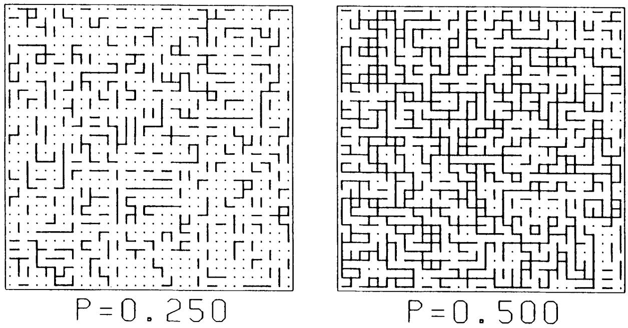

Fig. 2. Bond problem.

1990).

3) What are growth laws of clusters with increasing p, especially near above and below p_c? For example, it is known that the largest cluster size diverges as $\xi \sim (p_c\text{-}p)^{-\nu}$ for $p < p_c$ and the ratio of the sites contained in the largest cluster grows as $M \sim (p\text{-}p_c)^{\beta}$ for $p > p_c$ where ν and β are some fractional exponents. These are analogous to the critical phenomena in the phase transition problem. (Stauffer, 1985).

In spite of the simple presentation of the problem, rigorous analyses on these questions are hard works and little results are known yet. But the problem serves as an introductory exercise for the computer simulation and many accurate numerical results have been obtained.

Here let us try to introduce the topological consideration on the connectivity of the percolation clusters. However, the discrete lattice problems quoted above are unfitted for the topological consideration which is intrinsically a notion of continuity. Though a quantity which has a correspondence to the polygonal Euler characteristic (EC) has been used by pioneering researchers (Sykes and Essam, 1964), there is an obvious ambiguity on the dimensionality of clusters to be analyzed as is shown in Fig. 3. The value χ of EC of illustrated example depends on whether one regards it as a one dimensional graph ($\chi = -2$) or two dimensional one ($\chi = 1$). And for the extreme graph of fully occupied, i.e., fully connected state $p = 1$ which is as simplest as the empty state $p = 0$, one finds $\chi = -\infty$ (i.e. most complicated) as the former and $\chi = 1$ as the latter. In order to avoid this ambiguity one may reformulate the problem by packing problem with tiles or balls. Recently the specific EC is calculated analytically for a ball problem in arbitrary dimension. (Okun, 1990).

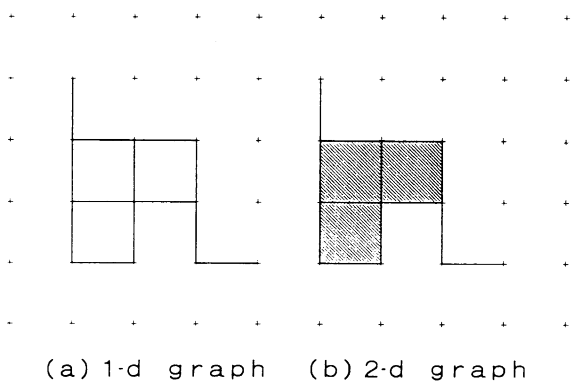

Fig. 3. Dimensionality of a given graph. The polygonal EC is –2 for (a) and 1 for (b).

Another choice is an excursion set of a stochastic random field. (Adler, 1980). Suppose water is poured into a random topography little by little, then ponds, lakes, seas and ocean would appear one by one. These are called excursion sets: Let $\{u(\boldsymbol{r})\}$ be a random field, i.e., a stochastic scalar variable defined at every point $\boldsymbol{r}$ in a d-dimensional Euclidean space $\mathcal{R}^d$. The excursion set and its boundary set are defined by

$$\mathcal{U} = \{\boldsymbol{r} | u(\boldsymbol{r}) < U\}, \tag{1}$$

and

$$\partial\mathcal{U} = \{\boldsymbol{r} | u(\boldsymbol{r}) = U\}, \tag{2}$$

respectively. Namely, $\mathcal{U}$ and $\partial\mathcal{U}$ denotes "sea" and "coast line" in the d-dimensional space. Note that if the random variable $u(\boldsymbol{r})$ at each point is completely independent, $\mathcal{U}$ cannot make any continuous sub-set of $\mathcal{R}^d$. In order to define some continuous object, i.e., manifolds in topological terms, spatial correlations are necessary. Then it is possible to define EC of $\mathcal{U}$ uniquely. The topological definition of EC is given by so-called Betti number which is a kind of characteristics of connectivity of spatial objects. Three dimensional examples are χ[a potato] = 1, χ[a doughnut] = 0, χ[a couple of contacted doughnuts] = −1, χ[a shell of nut] = 2, etc. For the present manifolds defined by Eq. (1) it makes explicit calculations easier to use algebraic definitions of EC. One is expressed with use of local curvatures of the closed boundary surface(s) $\partial\mathcal{U}$, i.e.

$$\chi[\mathcal{U}] = (2\pi)^{-1} \oint_{\partial\mathcal{U}} \kappa(a)\mathrm{d}a, \tag{3}$$

for $d = 2$, where da is the line element of the closed boundary curve $\partial\mathcal{U}$ and $\kappa(a)$ the curvature at each point on it, and

$$\chi[\mathcal{U}] = (4\pi)^{-1} \oint_{\partial\mathcal{U}} \kappa_1(a)\kappa_2(a)\mathrm{d}a, \tag{4}$$

for $d = 3$, where da is the area element of the closed boundary surface $\partial\mathcal{U}$ and $\kappa_1(a)$, $\kappa_2(a)$ are the principal curvatures at each point on it. These are the simplest cases of the Gauss-Bonnet theorem. Another algebraic definition is given by the Morse theorem. That is, EC is expressed by using the number of critical points $u(\boldsymbol{r}) = 0$ included in $\mathcal{U}$ as follows;

$$\chi[\mathcal{U}] = \sum_k (-1)^k \times \text{ number of rank } k \text{ critical points in } \mathcal{U}, \tag{5}$$

where the rank k indicates the number of negative eigenvalues of the matrix $\{\partial_i\partial_j u(\boldsymbol{r})\}$ at each critical point. Here $\partial_i u$ is an abbreviation for $\partial u/\partial x_i$. Thus the global index EC is calculable, at least in principle, within the local quantities only.

An explicitly tractable model is a correlated Gaussian field, whose probability density is given by

$$P(\{u(\boldsymbol{r})\}) \propto \exp\left[-\iint \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 u(\boldsymbol{r}_1) u(\boldsymbol{r}_2) / 2\sigma(|\boldsymbol{r}_1 - \boldsymbol{r}_2|)\right], \tag{6}$$

where the convariance $\sigma(\boldsymbol{r}_1, \boldsymbol{r}_2)$, i.e., the spatial correlation function of the field, is assumed to be translationally symmetric and isotropic. Though Eq. (6) is a continuously multi-variate normal distribution, the set of variables one needs in calculating the local quantities such as the curvature or the rank of critical point is merely $(u, \{\partial_i u\}, \{\partial_i\partial_j u\})$ at a single point. That is, the probability function Eq. (6)

is reducible to $1 + d + d(d + 1)/2$ dimensional normal distribution. (Tomita, 1989). Now the calculation becomes an elementary exercise of statistics. The result for the specific EC defined by $X_d(U) = \chi[\{\boldsymbol{r}|u(\boldsymbol{r}) < U\}]/V$ is very simple and is given by

$$X_d(U) = \lambda^{-d} H_{d-1}(-U)\exp\left(-U^2/2\right),$$
$$= \lambda^{-d}(\mathrm{d}/\mathrm{d}U)^d \phi(U), \tag{7}$$

where $H_n(x)$ is the usual Hermite polynomial (Tomita and Murakami, 1988) and

$$\phi(U) = (2\pi)^{-1/2}\int_{-\infty}^{U} \exp\left(-u^2/2\right)\mathrm{d}u, \tag{8}$$

which is used as the volume fraction of $\mathcal{U}$ in $\mathcal{R}^d$. For the simplicity the field amplitude is scaled by putting $\sigma(0) = 1$ without violating generality and a length scale $\lambda = (2\pi/\sigma''(0))^{-1/2}$ is used. Note that the expression Eq. (7) in these scales has a universal form, i.e., has no dependence on the detailed structure of the correlation function $\sigma(r)$ except for the correlation length defined as λ. A sample of the development of the "sea" for $d = 2$ with increasing U (or $\phi = \phi(U)$) is shown in Fig. 4.

The specific EC $X_d(U)$ is essentially the number density of isolated ponds (χ

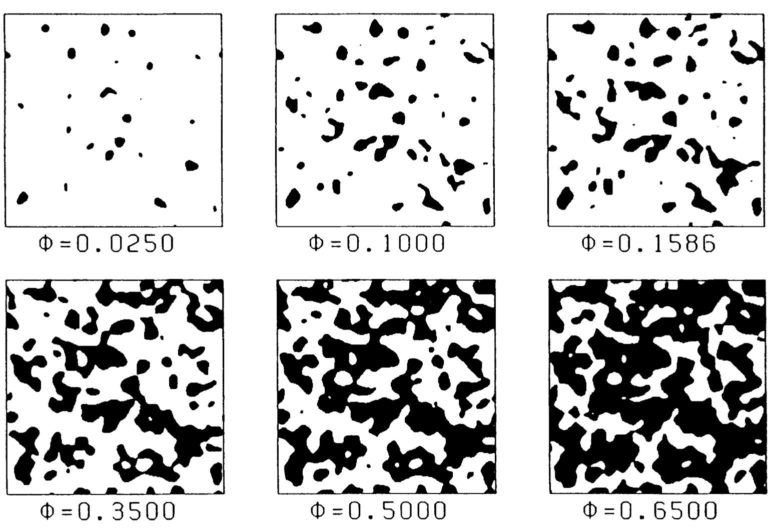

Fig. 4. Development of the "sea" in a Gaussian random field in $d = 2$.

= 1) for sufficiently small fraction ϕ. Then it is positive and increases with ϕ. It turns to decreasing at some value ϕ_M (= 0.15865··· for d = 2 and 0.04163··· for d = 3) due to coalescence of lakes. Note that self-coalescence of lake also decreases EC from χ[a lake] = 1 to χ[a lake with n islands] = 1 – n. Next it becomes negative above some critical fraction ϕ_c (= 0.5 for d = 2 and 0.15865··· for d = 3). The negative sign of EC means a percolating sea with many isolated islands in it for d = 2. Corresponding object in d = 3 is a percolating mesh structure of the 3·d sea. In this case, however, the 3·d land has a complementary mesh structure and is also percolating. Then there appears one more change of sign of the specific EC for d = 3 at $\phi = 1 - \phi_c = 0.84134\cdots$. The percolating sea becomes a foamy, sponge-like object with a positive EC and the complementary land is reduced to many isolated islands. In general one finds d – 1 sequential changes of sign for d-dimensional Euclidean space due to a property of the Hermite polynomials. This fact leads an intuitive expectation that there are d topological kinds of percolating structure including the fully occupied state ϕ = 1. In addition the first change of sign from positive to negative at $\phi = \phi_c$ should be the percolation threshold. Because of the self-similarity of the critically percolating graph, at least the mean topology should be invariant at ϕ_c for any scale transformation. One cannot find any point with such a property other than the zeros of $X_d(U)$. According to the above mentioned universality of the functional form of $X_d(U)$, the location of its zeros is invariant for any coarse-graining or smoothing transformation given by

$$\tilde{u}(\boldsymbol{r}) = \int K(\boldsymbol{r} - \boldsymbol{r}')u(\boldsymbol{r}')d\boldsymbol{r}', \tag{9}$$

which does not change the Gaussian nature of the field. In fact the explicit value ϕ_c = 0.15865··· (U_c = –1) for d = 3 is in good agreement with 0.16 obtained by a computer simulation (Skal *et al.*, 1973; Lebowitz and Saluer, 1986) and 0.157 given by a well-founded speculation from lattice problems (Zallen, 1983). The value U_c = –1 is also suggested in the famous textbook by Ziman (1979). And ϕ_c = 0.5 (U_c = 0) for d = 2 coincides with the exact value given by considerations on the symmetry of the field. Of course the trivial condition ϕ_c = 1 ($U_c = +\infty$) for d = 1 is satisfied. These values of the lowest zeros for different d are linked together by an analytic continuation as follows: Using the second expression of Eq. (7), one may extend the parameter d to a continuous one with an integral representation for fractional differential. The formula satisfying the boundary condition $X_d(-\infty) = 0$ is given by

$$X_{d-\nu}(U) = \Gamma(\nu)^{-1} \int_{-\infty}^{U} X_d(u)(U-u)^{-(1-\nu)}\mathrm{d}u, \quad (0 < \nu < 1) \tag{10}$$

where $\Gamma(\nu)$ is the Gamma function and the length scale λ is neglected for the simplicity. The sign of specific EC $X_d(U)$ thus extended to continuous d is shown as a phase diagram in Fig. 5. The lowest zone where $X_d(U) > 0$, the next where $X_d(U) < 0$ and the third where $X_d(U) > 0$ indicate the isolated lakes, the percolating mesh and the foamy object respectively, and so on.

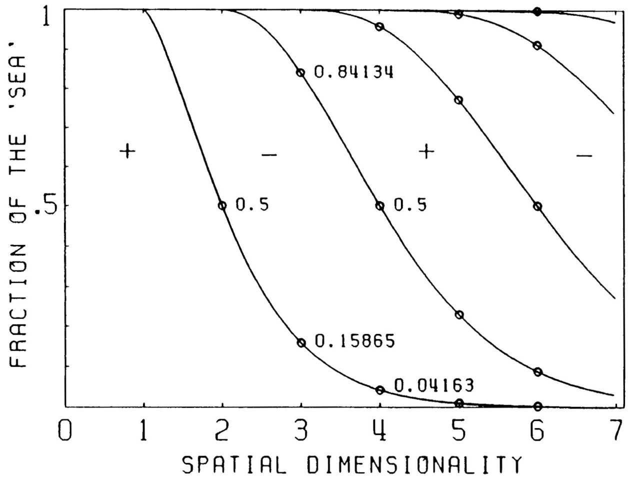

Fig. 5. A phase diagram for the specific EC.

The present work is originated in the non-equilibrium phase separation processes of binary mixtures. Similar works are found in the study of large scale structure of the universe (Melott, 1990).

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