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Can constrained percolation be approximated by Bernoulli percolation?

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Abstract

Many natural media can be regarded as essentially random while being partially determined, in the sense that their configuration and composition are subject to local deterministic constraints. These constraints, in general, affect a system's properties. Constraints can concern different levels and may be represented by geometric site constraints as well as by combinatorial ones. While they destroy independence and establish short-range correlations, it is suggested that constrained percolation systems may be approximated by independent percolation systems with appropriate interaction topologies.

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(Some figures in this article are in colour only in the electronic version)

A discrete medium can be represented by a (undirected) connected graph satisfying the following conditions: (a) the degree of every vertex is finite and (b) any finite subset of vertices contains at least one vertex which is adjacent to a vertex not contained in the subset. In the first approximation, a complex discrete medium can be regarded as a random graph. Random graph theory and percolation theory have provided many powerful tools to estimate topological properties of inherently random media. Thereby, analysis is often based on the assumption of stochastic independence of corresponding events. For example, a (Bernoulli) random medium is a medium in which the edges or vertices are open or occupied *independently* with some probability. While natural media exhibit a series of constraints, the assumption of independence is often too strong. Natural media might not be representable as Bernoulli media.

Constrained random systems often exhibit properties specific to their constraints. These properties and textures of the media will affect the dynamics running on it, particularly equilibrium states. For characterizing equilibrium states, measures induced by dynamics have

been mentioned and analysed in detail [7]. In this paper, we will mention random systems exhibiting constraints. Thereby we will focus on two classes of models: a class of random systems with *geometric site constraints*, i.e., media in which substructures are either given or forbidden, and a class of random systems with *state-dependent constraints*, i.e., those in which certain system states are given or forbidden.

This paper raises two questions. It is shown that constraints destroy stochastic independence and alter a system's properties. The lack of stochastic independence evokes serious mathematical problems and makes analysis difficult. The first question is whether a constrained percolation system can be approximated by an appropriate unconstrained one:

Can a constrained percolation system be approximated by an independent (Bernoulli) one?

Secondly, state-dependent constraints cause short-range correlations within the system, which alter the effective coupling topology in the system. This, in general, includes both the lattice type as well as the mode of next-neighbour interactions. This is shown by comparing our numerical estimates for particular state-dependent models with the results of independent percolation thresholds in various lattices with different interaction modes. This leads to the second question:

Given a constrained percolation system, can one predict the effective coupling topology of the approximating Bernoulli medium?

1. Constraints alter a system's properties

Constrained and unconstrained interacting particle systems may exhibit substantial differences concerning their macroscopic behaviour. This is well known from quantum mechanics, particularly for bosonic and fermionic systems. In fact, both systems differ in the existence of an exclusion rule which significantly alters particle distributions in state space. Their most impressive macroscopic difference concerns the phenomenon of the so-called *Bose–Einstein condensation* which means that the ground state becomes macroscopically occupied. While this is possible in bosonic systems, the exclusion principle prohibits this in fermionic systems.

1.1. Simple combinatorial constraints

For the sake of simplicity, we restrict ourselves to the (topologically) one-dimensional (1D) case in that we study the frequencies of events '*' and '-' in *constrained chains* (or Cayley trees). In a bicoloured chain, where '*' and '-' are chosen randomly and independently of each other with probabilities p and q = 1 - p, respectively, distributions are binomial. We now superimpose different constraints defined by

$$\mathcal{Y}_1 := (*, *),$$

 $\mathcal{Y}_2 := (*, -),$
 $\mathcal{Y}_3 := (-, -) \land (*, *)$

The requirement in model \mathcal{M}_i is that in the random chain the motif \mathcal{Y}_i must *not occur*. These constraints clearly destroy stochastic independence: whether a '*' can be added to a constrained chain may depend on the composition of the successive partial sequence. The process of prolongation therefore clearly is not Markovian. Further, as might be expected, distributions deviate from binomial. This is apparent from figure 1. Analysis is based on the well-known method of generating functions [3].



Figure 1. Distributions of events '*' and '-' in constrained chains. *q* is the probability for the event '-' and p = 1 - q is the probability for event '*'. Constraints chosen are, from left to right: $\mathcal{Y}_1 = (*, *), \mathcal{Y}_2 = (*, -)$ and $\mathcal{Y}_3 = (-, -) \land (*, *)$. Diagonals show the binomial distributions of events '*' and '-' in an unconstrained chain. Obviously, constraints evoke specific deviations from the binomial distribution. For example, due to the symmetry of the constraint $(-, -) \land (*, *)$ with respect to interchanging '*' and '-', the deviation is symmetrical to p = q = 1/2.

1.2. Geometrical site constraints

Exclusion principles may concern other system levels. While in the above example constraints were strictly local, geometric site constraints concern the requirement that the medium must, or, in the opposite, must not, contain a particular *structure*. Details and related analytical results can be found in [8].

When regarding the medium as a graph we can ask for all graphs $\mathcal{F}(H)$ on the given set of vertices which either do or do not possess a certain (weak) subgraph H. Evaluating the typical properties is closely related to counting. In general, counting is easy in situations where one can generate all objects in the set by a sequence of *independent* decisions in such a way that two different sequences never produce the same object. On the other hand, such site constraints destroy stochastic independence in general and, hence, make counting difficult. The strategy of overcoming this difficulty is called 'asymptotic enumeration'. Roughly speaking, the idea is to find an approximating subset $\mathcal{G} \subset \mathcal{F}(H)$ which contains almost all objects of the larger set and which can be generated by a sequence of independent decisions, such that good approximations for the cardinality of the dependent set under consideration can be obtained. The problem, of course, is to find an 'approximating' subset.

As an example, consider the set of all triangle-free graphs. This set cannot be generated by a sequence of independent decisions about whether an edge should exist or not, since the construction process is clearly not Markovian, i.e., depending on how earlier decisions are taken, later decisions are forced. The strategy of how to asymptotically enumerate trianglefree graphs is based on a fundamental observation which was proved by Erdös, Kleitman and Rothschild in 1976 [6].

Almost all triangle-free graphs are bipartite. [Erdös, Kleitman, Rothschild]

Therefore the set of all bipartite graphs is an approximating subset of the set of all triangle-free graphs. Constraints can lead to multiple phase transitions. Prömel and co-workers proved that *the evolution of the random triangle-free graph exhibits two phase transitions with respect to being bipartite*: first, for low edge density, the random triangle-free graph is almost surely bipartite, then it is not, and then it is once again. For detailed analysis, see [8]. This observation leads to the following natural question:



Figure 2. Two lattices, square SQ and triangular T, with their respective duals $SQ^* = SQ$ and H inscribed [4].

'Can a constrained medium be approximated by an independent (Bernoulli) one?'

To test this hypothesis we investigate various constrained percolation systems derived from two types of lattices, a triangular and a square lattice. Numerical estimates of the critical percolation thresholds suggest that constrained models can indeed be approximated by unconstrained ones, at least to some extent.

2. Percolation on constrained lattices

The general construction procedure of the models is as follows: consider an infinitely large lattice \mathcal{L} of particles (spins) and its dual \mathcal{L}^* . \mathcal{L} is randomly and independently bicoloured, i.e., particles *x* have states $\delta(x) \in \{1, -1\}$ with probabilities *p* and q = 1 - p, respectively. Each node *X* in \mathcal{L}^* corresponds to a *cell* of adjacent particles in \mathcal{L} . For example, if \mathcal{L} is a triangular lattice, a node in \mathcal{L}^* corresponds to a triangle in \mathcal{L} , while if \mathcal{L} is a square lattice, a node in \mathcal{L}^* corresponds to a triangle of a state $\zeta(X)$ to any cell, which in the simplest case is the sum of states of particles belonging to it, i.e.,

$$\zeta(X) := \sum_{i=0}^{m_{\mathcal{L}}} \delta(x_i).$$
⁽¹⁾

Again, if \mathcal{L} is a triangular lattice or a square lattice, then $m_{\mathcal{L}} = 3$ or 4, respectively. Obviously each node in \mathcal{L}^* can have states in $\Sigma = \{-m_{\mathcal{L}}, -m_{\mathcal{L}} + 2, \dots, m_{\mathcal{L}} - 2, m_{\mathcal{L}}\}$. Due to the construction, two neighbouring nodes in \mathcal{L}^* correspond to two adjacent cells in \mathcal{L} having a number of nodes in common. Hence, the states of neighbouring nodes in \mathcal{L}^* are not independent anymore. In contrast, they fulfil

$$|\zeta(X) - \zeta(X')| \leqslant \Delta_{\mathcal{L}}$$

where the constant depends on the lattice considered. In the case of the triangular lattice, we find $\Delta = 2$. A *motif* in this setting is a subset $C \subset \Sigma$. We say that a node $X \in \mathcal{L}^*$ is occupied if and only if $\zeta(X) \in C$.

Note that the strategy of implementing the constraint in the lattice is identical to above. The dual of a randomly and independently bicoloured lattice is coloured according to some rules defined by motifs. This corresponds to the idea that 'particular system substates must not occur'. In these models, this is clearly not a geometrical site but rather a state-dependent constraint. However, as usual we ask for the minimum probability that within the (infinite) lattice \mathcal{L}^* an infinite (open) cluster of occupied nodes exists given the constraint \mathcal{C} .

2.1. The constrained triangular lattice

The basic model was first described and analysed in some detail in [9]. The underlying triangular lattice is denoted by \mathcal{T} , while its dual honeycomb lattice is \mathcal{H} . There exist 14 non-trivial motifs. In this section, we particularly mention the case where no homogeneously coloured triangle in \mathcal{T} is allowed, i.e., a node $X \in \mathcal{H}$ is occupied only if its state fulfils

$$|\zeta(X)| = 1.$$

Hence, nodes in \mathcal{H} corresponding to 'unicoloured' triangles (1, 1, 1) or (-1, -1, -1,) are empty, i.e., not occupied. Other non-trivial motifs are analysed numerically in [1]. Obviously, the occupancy probability for a single node $X \in \mathcal{H}$ with $\zeta(X) = \pm 1$ is

$$S(p) = \mathbf{P}[X \text{occupied}] = \mathbf{P}[|\zeta(X)| = 1] = 3pq$$

where again $q = 1 - p, 0 \le p \le 1$. If nodes in \mathcal{H} were stochastically independent, the probability of finding two adjacent occupied nodes would be $S(p)^2$. This is, in fact, not true. In the opposite, the probability of finding two adjacent occupied nodes $X, X' \in \mathcal{H}$ is

$$P(p) = \mathbf{P}[X' \text{ occupied}, X \text{ occupied}] = 2p - 4p^3 - 2p^4$$

which is in fact larger than $S(p)^2$ for 0 . Using <math>P(p) as the effective occupancy probability we can evaluate the corresponding Cayley tree process for estimating the percolation threshold in \mathcal{H} . Hence there exist two threshold values for z = 3 determined by the solutions of the equation $P(p_c) = \frac{1}{2}$, i.e.,

$$p_c = 1 - \frac{1}{2}\sqrt{2} \approx 0.2928...$$
 and $\overline{p_c} = \frac{1}{2}\sqrt{2} \approx 0.7071...$

These values correspond nicely with the percolation thresholds observed in numerical simulations where $p_c \approx 0.2902$ and $\overline{p_c} \approx 0.7097$. The following observation was made in [9]:

The so-defined constrained site-percolation model on the triangular lattice can be approximated by independent bond percolation on a square lattice.

Hence, approximation may require both the choice of an appropriate lattice and of an appropriate interaction topology.

2.2. The constrained square lattice

We now consider constrained percolation on a square lattice SQ, which is self-dual, i.e., $SQ^* = SQ$. Obviously, each node $X \in SQ^*$ can have states in $\Sigma = \{-4, -2, 0, 2, 4\}$. Among all possible non-trivial motifs, we mention the following two, since their behaviour turned out to be most interesting. Furthermore, they are typical for all others, which lead to non-trivial percolation. The symmetric model S and the asymmetric A are defined as follows:

$$S = \{-2, 0, 2\}$$
 and $A = \{0, 2, 4\}.$

A node $X \in SQ^*$ is occupied if and only if $\zeta(X) \in S$ or A, respectively. Let $\pi^{\mathcal{C}}(p)$ be the occupancy probability for a single node due to constraint $\mathcal{C} \in \{A, S\}$. Then occupancy probabilities yield

$$\pi^{\mathcal{S}}(p) = 4p - 6p^2 + 4p^3 - 2p^4 \tag{2}$$

$$\pi^{\mathcal{A}}(p) = 6p^2 - 8p^3 + 3p^4 \tag{3}$$

such that critical percolation threshold(s) are implicitly determined by $\pi^{c}(p) = 0.5927460...$ In this case—the essential assumption being that events on SQ^* are *stochastically independent*—we would obtain

$$\pi_c^S = 0.201965\ldots$$
 $\overline{\pi}_c^S = 0.798035\ldots$ $\pi_c^A = 0.440106\ldots$

Since adjacent squares in *S* have two nodes in common, their states are not arbitrary but rather correlated. To investigate correlation between neighbouring nodes in SQ^* , we calculate the probability that two neighbouring nodes in SQ^* are occupied: let $P^{\mathcal{C}}(p)$ denote the effective occupancy probability of node *X* defined by

$$P^{\mathcal{C}}(p) := \mathbf{P}[\zeta(X) \in \mathcal{C}, \zeta(X') \in \mathcal{C}]$$

where *X*, *X'* are neighbours and *C* denotes the constraint, i.e., either C = A or C = S

$$P^{\mathcal{S}}(p) = 2p - 3p^2 + 6p^3 - 13p^4 + 12p^5 - 4p^6$$
⁽⁴⁾

$$P^{\mathcal{A}}(p) = p^2 + 4p^3 - 2p^4 + p^6.$$
⁽⁵⁾

To estimate threshold values in the constrained system, we use the *mean field approximation*. The correlation function, i.e., the probability of finding a constrained chain of length ℓ , yields

$$G_{\ell}^{\mathcal{C}}(p) = \frac{z}{z-1} ((z-1)P^{\mathcal{C}}(p))^{\ell}$$

It follows for the square lattice, i.e., z = 4, that thresholds are implicitly determined by $\frac{1}{z-1} = P^{\mathcal{C}}(p_c^{\mathcal{C}})$, such that

$$p_c^{S} = 0.2194...$$
 $\overline{p}_c^{C} = 0.7806...$ $p_c^{A} = 0.3838...$

These values should be compared with those obtained from *numerical simulations*. We first considered the random growth of a cluster in SQ by successively adding adjacent occupied vertices or shells to the cluster. Below, we list the threshold values estimated numerically by considering *constrained spreading site percolation* under periodic boundary conditions on square lattices up to size 1024×1024 , while the sample size is up to 1200 per point and step-width down to 2.5×10^{-4} around the critical value:

$$\mathbf{p}_{c}^{S} = 0.1970(8) \dots$$
 $\overline{\mathbf{p}}_{c}^{S} = 0.8029(2)$ $\mathbf{p}_{c}^{A} = 0.4072(8) \dots$

Critical percolation thresholds have been extrapolated from averaged results obtained by firstpercolation-scans, described in [10]. For comparison, we also estimated threshold values from numerical simulations of *constrained geometrical (orthodox) site percolation* on square lattices for fixed boundary conditions up to size 3200×3200 with sample size 2500 to obtain $\mathbf{p}_c^S \approx 0.196(7)$ and $\mathbf{p}_c^S \approx 0.4070(1)$ [1].¹ These values are summarized in table 1.

For the asymmetric A-model, a clear shift to the left is predicted and, in fact, observable, i.e., percolation is reached earlier due to positive correlation between events. While a similar shift might be expected for the symmetric model also, there is no clear numerical evidence for it. This finding is supported by (one-dimensional) analysis of correlation length (unpublished results by Tupak) and also by the data concerning lacunarity, see below.

¹ Using the same method as Bendisch (maximum of the discrete derivation) to evaluate \mathbf{p}_c , we obtained $\mathbf{p}_c^S = 0.1956(7)$ and $\mathbf{p}_c^A = 0.4071$.



Figure 3. Lacunarity as a function of the occupation density $\rho_C(p)$ defined in SQ^* for three models of spreading percolation on the square lattice, model A, model S and the independent model. Textures of corresponding media, characterized by their lacunarity, differ significantly. Again, the symmetric model shows strong similarities with the unconstrained one.

Table 1.				
Constrained SQ	p_c Bernoulli	p_c numerical	p_c mean field	
\mathcal{S} -model \mathcal{A} -model	0.202 0.440	0.197 0.407	0.219 0.384	

2.3. Constraints may affect texture

For the models considered above, critical exponents coincide with those in Bernoulli percolation (unpublished results by Tupak) and, hence, do not show the effects of short-range correlations imposed by constraints. Nevertheless, the effects of local constraints should leave some 'blue prints' in the constrained medium. The idea behind this is to consider the texture of the constrained medium, measured by its 'lacunarity'. The main question was whether the constrained models \mathcal{A} and \mathcal{S} produce the same lacunarity as the Bernoulli model.

Constraints introduce short-range correlations between events in the media. While these short-range correlations are covered near the critical point, it is expected that they cause effects on shorter scales. These constraints should show up in the texture of the medium. To characterize texture, we estimated the following quantity, often called *lacunarity*:

$$\mathbf{L}^{\mathcal{C}}(\rho) := \frac{\Delta \mathcal{M}^{\mathcal{C}}(\rho)^2}{\langle \mathcal{M}^{\mathcal{C}}(\rho) \rangle^2} \tag{6}$$

where $\rho = \rho_C(p)$ is the density of occupied nodes in the respective dual lattice subject to constraint *C* and $\mathcal{M} = \mathcal{M}^C(\rho)$ is the cluster mass in model *C* at ρ . Further, $\Delta \mathcal{M}^2 = \langle (\mathcal{M} - \langle \mathcal{M} \rangle)^2 \rangle$. This value can be regarded as a measure for the size of fluctuations of the cluster mass around its mean. Hence in a homogeneous medium \mathcal{L} is 0. The larger \mathcal{L} is, the more the medium deviates from being homogeneous.

Figure 3 shows this entity for independent site percolation and the constrained media subject to constraints A and S as a function of the occupancy density ρ^{c} in the constrained

system. Simulations were conducted on a square lattice of size 1024×1024 with sample sizes of 10^6 for constraint A, 7.5×10^5 for S, and 6×10^5 for independent percolation. It is apparent that the three media have different textures in the subcritical regime.

This may be interpreted as follows: while the masses of percolating clusters in the three models are the same for ρ_c larger than the critical density, the respective media are homogeneous. Lacunarity increases when ρ^c tends to the critical occupancy probability ρ_c^c . Further, $\mathbf{L}^A(\rho^c) > \mathbf{L}(\rho^c)$ for $0 < \rho^A < \rho_c^A$. Hence for $\rho^A < \rho_c^A$, i.e. subcritical, the A medium is more heterogeneous than the unconstrained one, i.e. mass fluctuations here are larger. According to its larger lacunarity, the A medium is regarded as exhibiting larger blobs/holes in the cluster of the same mass than in the independent model, so that the cluster mass distribution is altered. This then leads to a lower percolation threshold, as is, in fact, observed. According to this picture, we also suggest that the S medium has a slightly lower p_c than the unconstrained medium, which is also in agreement with our numerical results.

3. Constraints alter effective coupling topologies

We studied a set of particular constrained random systems. The constraints considered are geometric site constraints and combinatorial or state-dependent constraints. In any case, it was shown that constraints significantly altered the systems's behaviour. Constraints may not only lead to shifts in critical percolation probabilities, but also result in establishing multiple thresholds. Moreover, constraints establish short-range correlations. They may alter the effective coupling topology in the medium in that interaction then is not restricted to next neighbours only, rather, it involves others. The symmetric model in the square lattice case is special in this respect. On the one hand, one would expect a clear shift in the percolation thresholds, which in fact can only just be seen. Moreover, mean field analysis shows that at the threshold value, correlations between nodes do vanish so that at the critical point the medium 'looks' Bernoulli. Anyway, our conjecture is that constraints, in general, alter the effective lattice type. There is further evidence for this suggestion.

As reported in [5], the critical percolation threshold in a triangular lattice with secondneighbour interaction is $p_c = 0.289$, which is close to our numerically estimated value $p_c = 0.2902$. Further, the two models for constrained percolation on the square lattice have threshold values $p_c^A = 0.407$ and $p_c^S = 0.197$. These values may be compared with those of independent site percolation on a square lattice with *m*-neighbour interaction: the percolation threshold $p_c^{(m)}$ in a square lattice with *m*-neighbour interaction is

$$p_c^{(2)} = 0.404$$
 to be compared with $p_c^{\mathcal{A}} = 0.407$
 $p_c^{(4)} = 0.195$ to be compared with $p_c^{\mathcal{S}} = 0.197$.

This then leads to the more general question whether a particular constrained system on some lattice can be approximated by independent percolation on an appropriate lattice with specific *m*th neighbour interaction. In fact, this seems to be the case. In [1], the threshold values of all 14 non-trivial models on a triangular lattice were estimated. Let $\mathbf{p}_c^{(M)}$ be the percolation threshold in the constrained model *M*. It turned out that there exist only four fundamental percolation models, i.e., all others can be deduced from only these four. Corresponding models are (-3, -1), (-1, +1), (+1, +3), (-3, +3), where a node in \mathcal{T}^* in model (-1, +1), for example, is occupied if it contains either two +1 spins and one -1 spin, or two -1 spins and one +1 spin. These values should be compared with the following.

There are 11 regular lattices in the plane, i.e., the Archimedean Tillings. Among them are the 6-regular triangular lattice 3^6 , the two 5-regular lattices $(3^3, 4^2)$ and $(3^2, 4, 3, 4)$ and the 4-regular square lattice 4^4 . Now let $p_c^{\tau,m}$ denote the critical percolation probability in

independent site percolation on the lattice of type τ with *m*-neighbour interaction. Here, τ is the lattice type index, i.e., $\tau \in \{3^6, (3^3, 4^2), (3^2, 4, 3, 4), 4^4\}$. The following coincidence of the corresponding percolation values with our fundamental models, see above, is intriguing:

$\mathbf{p}_c^{(-3,3)} = 0.215(4)$	\longleftrightarrow	$p_c^{3^6,3} = 0.215$	
$\mathbf{p}_c^{(-1,1)} = 0.290(2)$	\longleftrightarrow	$p_c^{3^6,2} = 0.289$	$p_c^{4^4,3} = 0.289$
$\mathbf{p}_c^{(-3,-1)} = 0.459(7)$	\longleftrightarrow	$p_c^{(3^2,4,3,4),2} = 0.442$	$p_c^{(3^3,4^2),2} = 0.446$
$\mathbf{p}_c^{(1,3)} = 0.540(2)$	\longleftrightarrow	$p_c^{(3^2,4,3,4),1} = 0.550$	$p_c^{(3^3,4^2),1} = 0.548.$

Irrespective of the numerical coincidence, it should be kept in mind that one set of threshold values is for the constrained systems in which the events are correlated rather than independent, while in the other class the events are independent. Particularly, in the symmetric (-1, 1) we have two threshold values symmetric to 1/2, a phenomenon which does not exist in the independent 3^6 , 2 and 4^4 , 3 models.

These coincidences should be taken seriously in the following sense: as mentioned in section 2, a constrained model may be well approximated by an appropriate independent one: the set of triangle-free graphs was approximated by the set of bipartite graphs. The above results suggest that particular constrained models could be approximated by independent models with appropriate (interaction) topology: for example, model (-3, -1) on the triangular lattice might be approximated by independent site percolation on a 5-regular lattice second- or third-neighbour interaction. However, one should be cautious about interpreting the similarity of threshold values of two models with respect to the identity of these two models.

Further numerical and analytical considerations are necessary to judge the reasonability of the idea that a constrained percolation model can be approximated by an appropriate independent percolation model. Moreover, the task is the following. *Given a constrained percolation system, predict the effective lattice topology of an approximating independent model from the knowledge of constraints.*

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