Selective bootstrap percolation

Mauro Sellitto

Dipartimento di Ingegneria, Università degli Studi della Campania ‘Luigi Vanvitelli’, Via Roma 29, 81031 Aversa, Italy
The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, 34151 Trieste, Italy
E-mail: mauro.sellitto@unicampania.it and mauro.sellitto@gmail.com

Received 4 August 2019
Accepted for publication 16 September 2019
Published 7 November 2019

Abstract. A new class of bootstrap percolation models in which particle culling occurs only for certain numbers of nearest neighbours is introduced and studied on a Bethe lattice. Upon increasing the density of initial configuration they undergo multiple hybrid (or mixed-order) phase transitions, showing that such intriguing phase behaviours may also appear in fully homogeneous environments, provided that culling is selective rather than cumulative. The idea immediately extends to facilitation dynamics, suggesting a simple way to construct one-component models of multiple glasses and glass-glass transitions as well as more general coarse-grained models of complex cooperative dynamics.

Keywords: percolation problems, classical phase transitions, dynamical processes
Introduction

Bootstrap percolation (BP) is a primary example of a statistical mechanics model in which a discontinuous phase transition is accompanied by critical fluctuations \cite{1}. Interest in this unusual hybrid (or mixed-order) phase behaviour has grown in the last few years while it has been discovered in a variety of quite unrelated systems \cite{2, 3} \cite{1}. Prominent examples of interest here are certain models of complex networks \cite{4–6}, and especially of glassy systems, where the possibility of multiple hybrid phase transitions and higher-order singularities \cite{7–9}, similar to those first discovered in the mode-coupling theory \cite{10, 11}, was inferred through the close connection of BP with facilitation glassy dynamics \cite{12, 13}. These results were generally obtained at the price of introducing some form of inhomogeneity in the problem, such as a fluctuating connectivity in the underlying lattice structure or multiple culling thresholds \cite{4–9}, according to which a particle is culled if a cumulative constraint on the number of its nearest neighbours is satisfied in the form of inequality (less than or, equivalently, greater than). In this paper, we show that this inhomogeneity is not a necessary ingredient and one may find multiple hybrid phase transitions in fully homogeneous environments provided that particle culling is selective, i.e. it does involve only certain specific numbers of nearest neighbours.

There are two main general motivations behind this work. The first stems from the difficulty of finding one-component schematic models of multiple glasses which are sufficiently simple to allow for large scale numerical simulations or even analytical solutions of their equilibrium and aging dynamics. Multiple hybrid phase transitions in such systems, generally arise from the presence of two (or more) microscopic length scales (typically a repulsive hard-core plus a short-range attractive or even repulsive potential) \cite{14–18}. It is the competition between these length scales that leads, as the thermodynamic control parameters are changed, to multiple phases dominated by qualitatively different particle packing mechanisms on different length scales.

The second motivation is that the idea put forward here may be useful, more broadly, for understanding certain forms of complex dynamics in which cooperativity...

\footnote{Bar and Mukamel \cite{3}; and references therein for early examples of mixed-order phase transitions in one dimensional spin models with long-range interactions.}
does not necessarily involves a cumulative effect but rather a selective one. It is well
known, for example, that many soft matter systems dominated by hydrophobic inter-
actions [19], most notably proteins, lose their biological functionality when thermo-
dynamics variables (temperature, pressure, pH concentration) lie outside a relatively
narrow range around their ambient values, leading to unusual reentrant Tammann
phase diagrams [20–23]. Another example of interest is offered by the evolutionary
dynamics of ecological systems whose stationary states are typically neither scarcely
populated nor overcrowded, as epitomized by the celebrated Game of Life cellular
automaton, whose dynamical rules are strongly reminiscent of selective kinetic con-
straints, albeit of irreversible type [24, 25].

Bootstrap percolation

BP is generally concerned with the statistical properties of particle clusters generated
on a lattice according to the following procedure. The sites of a lattice with coordi-
nation number $k + 1$ are first occupied with probability $p$ as in ordinary percolation.
Then, particles with at least $f$ vacant neighbours are iteratively removed one by one,
until a static configuration is reached\(^2\). Depending on $p$, the final configuration can
either be empty or contain an $f$-cluster built up by particles with less than $f$ vacant
neighbours. The passage between these two states may have intriguing critical features.
On locally tree-like lattices with fixed branching ratio $k$, the case we consider here, an
infinite $f$-cluster can only exist for $f > 1$ and the BP problem can be solved exactly [1].
The residual fraction, $\Phi$, of occupied site represents the system order parameter and
can be written as:

$$
\Phi = p \sum_{i \in S} \binom{k + 1}{i} B^i (1 - B)^{k+1-i},
$$

where $S = \{0, 1, \ldots, f - 1\}$ is the set of numbers of nearest neighbours that prevent
particle culling, and $B$ is the probability that a site is not connected to the infinite $f$-clus-
ther through a nearest neighbour, which obeys the self-consistent polynomial equation:

$$
1 - B = p \sum_{i \in S} \binom{k}{i} B^i (1 - B)^{k-i}.
$$

The critical properties of BP transitions are easily established by Taylor expanding the
right member side of equation (2) in powers of $1 - B$. The presence of a linear term
for $f = k$ implies a continuous phase transition located at $p_c = 1/k$. The incipient span-
ning $f$-cluster in this case is fractal, as the model reduces to the usual random perco-
lation. When $1 < f < k$, instead, the absence of a linear term in $1 - B$ implies that $B$, and therefore $\Phi$, must change abruptly: the phase transition is discontinuous and the

\(^2\) Note that our definition of the bootstrap percolation rule is equivalent, on the regular lattice considered here, to
the one traditionally used in the literature, in which a particle is culled if it has less than $m = k - f + 2$ neigh-
bouring particles. This is done with the purpose of making a more direct connection to works on facilitated glassy
dynamics in which a spin can flip only when it has at least $f$ nearest neighbouring down-spin state.
structure of the \( f \)-cluster is compact. However, since \( \Phi \) has a square root singularity at the transition the diverging susceptibility \( d\Phi/dp \) implies critical fluctuations. The underlying geometrical nature of this behaviour is the diverging mean size of corona clusters (i.e. clusters in which every particle has exactly \( f-1 \) vacant neighbours) and their structural fragility (corona collapse occurs, as in domino-like games, by a single particle culling) [5].

Selectively bootstrap percolation

In the more general selective bootstrap percolation (SBP) we now introduce, \( \mathcal{S} \) is an arbitrary subset of non-negative integers less than \( f \). The critical properties of the phase transition first encountered by increasing \( p \) is determined by the lowest order terms in \( 1-B \) of the equation \( Q = 0 \), with:

\[
Q(B) = 1 - B - p \sum_{i \in \mathcal{S}} \binom{k}{i} B^i (1-B)^{k-i},
\]

which depends only on the maximum value of \( \mathcal{S} \), that is \( \max \mathcal{S} = f-1 \). Therefore we fully recover the two types of phase behaviour previously discussed for BP: a continuous transition located at \( p_c = 1/k \) when \( \max \mathcal{S} = k-1 \), and a discontinuous hybrid transition for \( 2 \leq \max \mathcal{S} < k-1 \). From a purely mathematical point of view, the main novelty of SBP is that, when gaps in the sequence of non-negative integers less than \( f \) are generally allowed, the absence of some powers of \( B \) in the polynomial \( Q(B) \) will possibly lead to the appearance of extra real roots and, consequently, to multiple hybrid phase transitions. From a more physical point of view, the selective kinetic constraint allows for the formation of different corona clusters, whose competition and stability lead to the existence of multiple hybrid behaviour, as the density of the initial particle configuration is changed. Moreover, by simply increasing the lattice connectivity one can further augment the number of real roots (up to \( k \), virtually, by the fundamental theorem of algebra). Therefore, we can generally conclude that SBP displays a phase behaviour richer than BP, even though the basic geometric mechanism of the hybrid behaviour in SBP remains essentially the same as that of BP.

Before illustrating explicitly these results in two cases, it is important to emphasize that the correct determination of the phase diagram and the evolution of the order parameter \( \Phi \) in the presence of multiple phase transitions, requires that a stability criterion for the selection of the physical stable solution is properly established. This is simply done by observing that: (i) the particle fraction \( \rho_t \) populating the lattice at time \( t \), while particle culling is carried out, is a non-increasing function of \( t \), and (ii) the asymptotic density \( \rho_\infty = \Phi \) is a monotonic increasing function of the initial particle fraction \( \rho_0 = p \). This implies that the stable physical solution corresponds to the value of the residual fraction \( \Phi \) or, equivalently, \( B \), which is first encountered during culling dynamics, namely to the largest root of equation (3).

The first case we consider is a Bethe lattice with branching ratio \( k = 7 \) and \( \mathcal{S} = \{0, 1, 2, 5\} \) which gives the self-consistent equation:

https://doi.org/10.1088/1742-5468/ab47fa
As shown in figure 1 the potential $Q$ has two real roots. Accordingly, the order parameter $\Phi$ undergoes two jumps with a square-root singularity (the first located at $p_I^c \approx 0.7046...$ and the second at $p_{II}^c \approx 0.9149...$) implying critical fluctuations and therefore a double hybrid phase transition, as expected (since $\max S = 5 < k = 1 - 6$).

Next we consider the set $S = \{0, 1, 2, 3, 6\}$ for a Bethe lattice with $k = 7$. This gives the self-consistent equation:

$$1 - B = p \left[(1 - B)^7 + 7(1 - B)^6 B + 21(1 - B)^5 B^2 + 21(1 - B)^2 B^7\right].$$  \hspace{1cm} (4)

As shown in figure 1 the potential $Q$ has two real roots but now the order parameter $\Phi$ undergoes first a continuous phase transition at $p_I^c = 1/7 \approx 0.1437...$ (as expected, since $\max S = 6 = k - 1$), and then a hybrid phase transition located at $p_{II}^c \approx 0.7986...$

To highlight the fold (or, equivalently, saddle-node) bifurcation of the discontinuous transition we show, in the right panel of both figures 1 and 2, the unstable and metastable solutions. The former corresponds to the order parameter decreasing with $p$, which clearly violates the condition $(ii)$ of the stability criterion of physical solution previously discussed. The latter, also violates that criterion, nevertheless, in facilitation dynamics closely related to BSP, the observation of metastable solutions in out of equilibrium states, e.g. during a sufficiently slow annealing and for suitable initial conditions, is possible.

Finally, it should be noticed that although the number of jumps in the order parameter can be increased by introducing additional gaps in the sequence of integers of $S$ and making $k$ larger, the absence of a continuously tunable parameter makes it difficult to find $A_{\ell}$ bifurcation singularities (at which the order parameter critical exponent is $\beta = 1/\ell$). The appearance of such higher-order critical points, corresponding to an $\ell$-degeneracy ($\ell \geq 2$) of the largest root of $Q$, that is:

$$\frac{d^n Q}{dB^n} = 0, \quad n = 0, \ldots, \ell - 1,$$  \hspace{1cm} (6)

with the $\ell$th derivative being nonzero, though $a \text{ priori}$ not impossible for suitable values of $k$ and $S$, must be considered rather accidental.
Conclusions

To conclude, we have introduced a simple and rather straightforward modification of BP featuring multiple hybrid phase behaviour on a random regular graph with fixed connectivity (i.e. a Bethe lattice), in a fully homogeneous environment. We expect this extension of the BP framework to be relevant to the field of complex networks and other forms of cooperative dynamical problems. In particular, the connection between BP and facilitation dynamics immediately suggests how to construct cooperative models with selective facilitation: a non-interacting spin system in which a spin can flip only when the number of its down-spin nearest neighbours belongs to the set $S$, will have a relaxation dynamics with multiple phases corresponding to the fixed points of SBP equation (2). A similar procedure also applies to kinetically constrained particle models. By exploiting this connection one could address the relaxation dynamics of multiple glasses, a problem that seems at the moment hardly affordable in mean-field disordered $p + q$-spin models, as the one-step replica symmetry breaking solution seems to be unstable in this type of systems [26, 27]. Also, it would be interesting to investigate, e.g. with the $M$-layer construction [28], how multiple glass transitions are possibly avoided in physical dimension [29, 30]. This might shed some light on the nature of ergodicity breaking in multiple glasses observed experimentally and numerically in short-range attractive colloids and related systems [15–17].

Acknowledgments

This work was partly supported by the Italian Ministry of Instruction, University and Research (MIUR) through Grant FFABR 2017.

References

[1] Chalupa J, Leath P L and Reich G R 1979 Bootstrap percolation on a Bethe lattice J. Phys. C: Solid State Phys. 12 L31
[2] For a review, see: De Gregorio P, Lawlor A and Dawson K A 2009 Encyclopedia of Complexity and Systems Science ed R A Meyers (New York: Springer) pp 608–26

https://doi.org/10.1088/1742-5468/ab47fa
Selective bootstrap percolation

[3] Bar A and Mukamel D 2014 Mixed-order phase transition in a one-dimensional model Phys. Rev. Lett. 112 015701
[4] Branco N S 1993 Probabilistic bootstrap percolation J. Stat. Phys. 70 1035
[5] Baxter G J, Dorogovtsev S N, Goltsev A V and Mendes J F F 2010 Bootstrap percolation on complex networks Phys. Rev. E 82 011103
[6] Cellai D, Lawlor A, Dawson K A and Gleeson J P 2011 Tricritical point in heterogeneous k-core percolation Phys. Rev. Lett. 107 175703
[7] Sellitto M, De Martino D, Caccioli F and Arenzon J J 2010 Dynamic facilitation picture of a higher-order glass singularity Phys. Rev. Lett. 105 265704
[8] Sellitto M 2012 Cooperative heterogeneous facilitation: multiple glassy states and glass-glass transition Phys. Rev. E 86 030502
[9] Parisi G and Sellitto M 2015 The large-connectivity limit of bootstrap percolation Europhys. Lett. 109 350401
[10] Dawson K, Foffi G, Fuchs M, Götze W, Sciortino F, Sperl M, Tartaglia P, Voigtmann T and Zaccarelli E 2000 Higher-order glass-transition singularities in colloidal systems with attractive interactions Phys. Rev. E 63 011401
[11] Götze W 2009 Complex Dynamics of Glass-Forming Liquids (Oxford: Oxford University Press)
[12] Ritort F and Sollich P 2003 Glassy dynamics of kinetically constrained models Adv. Phys. 52 219
[13] Sellitto M, Biroli G and Toninelli C 2005 Facilitated spin models on Bethe lattice: bootstrap percolation, mode-coupling transition and glassy dynamics Europhys. Lett. 69 496
[14] Sciortino F 2002 Disordered materials: one liquid, two glasses Nat. Mater. 1 145
[15] Pham N, Puertas A M, Bergenholtz J, Egelhaaf S U, Moussaïd A, Pusey P N, Schofield A B, Cates M E, Fuchs M and Poon W C 2002 Multiple glassy states in a simple model system Science 296 104
[16] Voigtmann Th 2011 Multiple glasses in asymmetric binary hard spheres Europhys. Lett. 96 36006
[17] Guan N, Das G, Sperl M, Sciortino F and Zaccarelli E 2014 Multiple glass singularities and isodynamics in a core-softened model for glass-forming systems Phys. Rev. Lett. 113 258302
[18] Maimbourg T, Sellitto M, Seremjian G and Zamponi F 2018 Generating dense packings of hard spheres by soft interaction design SciPost Phys. 4 039
[19] Nelson P 2004 Biological Physics (New York: WH Freeman)
[20] Greer A L 2000 Too hot to melt Nature 404 134 (and references therein)
[21] Stillinger F H and Debenedetti P G 2003 Phase transitions, Kauzmann curves and inverse melting Biophys. Chem. 105 211
[22] Schupper N and Shnerb N M 2005 Inverse melting and inverse freezing: a spin model Phys. Rev. E 72 046107
[23] Plasser G et al 2006 Crystallization on heating and complex phase behavior of α-cyclodextrin solutions J. Chem. Phys. 125 154504
[24] Schulman L S and Seiden P E 1978 Statistical mechanics of a dynamical system based on Conway’s game of life J. Stat. Phys. 19 203
[25] Bagnoli F, Rechtman R and Ruffo S 1991 Some facts of life Physica A 171 249
[26] Krakoviack V 2007 Comment on spherical 2+p spin-glass model: an analytically solvable model with a glass-to-glass transition Phys. Rev. B 76 136401
[27] Crisanti A and Leuzzi L 2007 Reply to Comment on spherical 2+p spin-glass model: an analytically solvable model with a glass-to-glass transition Phys. Rev. B 76 136402
[28] Rizzo T 2019 Fate of the hybrid transition of bootstrap percolation in physical dimension Phys. Rev. Lett. 122 108301
[29] Rizzo T and Voigtmann Th 2019 Solvable models of supercooled liquids at the avoided mode-coupling-theory transition (arXiv:1903.01773)
[30] Parisi G and Rizzo T 2008 K-core percolation in four dimensions Phys. Rev. E 78 022101

https://doi.org/10.1088/1742-5468/ab47fa