Changeover phenomenon in randomly colored Potts model

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The Hybrid Potts (HP) model

- Consider a Potts Hamiltonian $\mathcal{H}(\{\sigma\})$ where $\{\sigma\}$ is a configuration of N spins, each can select one out of $\{1, 2, ..., Q_i\}$ colors where

$$Q_i = -X_i(q - q_0) + q, \; i = 1, ..., N \; , \tag{1}$$

  and $X_i \sim \mathrm{Ber}(p)$ are *i.i.d.* random variables.
- Let q_c be the maximal integer for which the transition is continuous. Each spin can be colored by $q_0 \leq q_c$ "strong" colors with probability p and by $q > q_c$ colors (containing $q - q_0$ additional "weak" colors), with probability $1 - p$.
- Spins chosen with probability p or $1 - p$, belong to strong or weak regions, respectively.

Main result

There is a marginal concentration p^* such that the transition is is discontinuous for $p < p^*$ and continuous for $p \geq p^*$.

The standard HP model

- *Simple* clusters, growing sub-exponentially with their size, have a minimal number of sites per bond, i.e., $1/2 + o(1)$.
- Fractals have $1/2 + \delta + o(1)$ ($\delta \leq 1/2$) sites per bond. Let $\#(k, n)$ be the number of fractals with n sites such that k of them are positioned in strong regions. The expected number of such fractals is

$$\langle \#(k, n) \rangle = \mu^n \binom{n}{k} p^k (1 - p)^{n-k} \; , \tag{2}$$

  where $\sum_k \#(k, n) \sim \mu^n$ and $\mu \equiv \mu(\delta)$ is the growth constant of those fractals [1].
- The expected change in the number of states is given by $\langle \#(k, n) \rangle q_0^{-k} q^{-(n-k)}$.
- Assuming that $\#(k, n)$ is narrowly distributed around its mean, the free energy per site can be written as

$$-\beta f_{\mathrm{frac}} = \frac{2\beta}{1 + 2\delta} + \ln \mu - \ln q + \sum_k \left(\frac{1}{n} \ln \left(\binom{n}{k} p^k (1 - p)^{n-k} \right) + \frac{k}{n} \ln \left(\frac{q}{q_0} \right) \right) \; . \tag{3}$$

- In the large n limit, the sum in (3) can be replaced with the maximum of the summand obtained at k satisfying

$$\kappa = \frac{pq}{pq + (1 - p) q_0} \; , \tag{4}$$

  with $\kappa = k/n$. This brings (3) into the form

$$\begin{aligned} -\beta f_{\mathrm{frac}} &= \frac{2\beta}{1 + 2\delta} + \ln \mu - \ln q \\ &- \kappa \ln \kappa - (1 - \kappa) \ln(1 - \kappa) + \kappa \ln p + (1 - \kappa) \ln(1 - p) + \kappa \ln \left(\frac{q}{q_0} \right) \; . \end{aligned} \tag{5}$$

- The free energy per site of simple clusters is given by

$$-\beta f_{\mathrm{sim}} = 2\beta - p \ln q_0 - (1 - p) \ln q \; . \tag{6}$$

- If at β solving $f_{\mathrm{sim}} = 0$ we have $f_{\mathrm{frac}} \geq 0$, then it is disadvantageous for the system to occupy fractals at that temperature $\Longrightarrow$ first order transition at

$$\beta_c \approx \frac{1}{2} (p \ln q_0 + (1 - p) \ln q) \; . \tag{7}$$

- The concentration p^* is estimated by taking κ^* to satisfy (4) at p^*, plugging it into (5) together with the RHS of (7) and solving

The standard HP model

$$\sup_{\delta} \Big(p^* \ln q_0 + (1 - p^*) \ln q + (1 + 2\delta) \times \Big(\ln \mu - \ln q - \kappa^* \ln \kappa^* - (1 - \kappa^*) \ln(1 - \kappa^*) + \kappa^* \ln p^* + (1 - \kappa^*) \ln(1 - p^*) + \kappa^* \ln(q/q_0) \Big) \Big) = 0 \; , \tag{8}$$

for p^*.

- The large q behavior is then given by

$$p^* \sim \frac{\ln q}{q} \; . \tag{9}$$

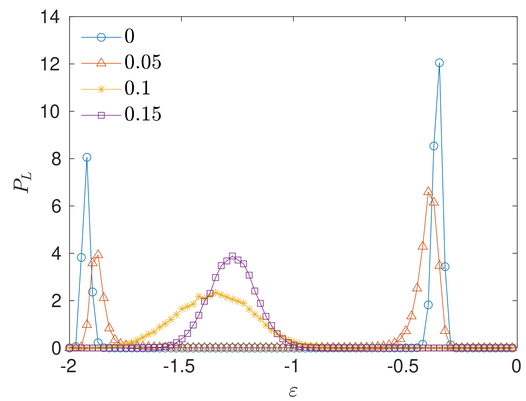


Figure 1. Energy PDF for the standard model with spin numbers $q_0 = 2$ and $q = 50$. The lattice linear size is $L = 40$. The concentration p^* is expected to be $0.05 \leq p^* < 0.15$, in reasonable agreement with (9) yielding $\frac{\ln 50}{50} \simeq 0.08$.

The mean field (MF) HP model

- The MF Hamiltonian is given by

$$\mathcal{H}_{MF} = -\frac{1}{N} \sum_{i<j} \delta_{\sigma_i, \sigma_j} \; . \tag{10}$$

- Let ξ_i and η_i be the fraction of spins with color $i \in \{0, 1, ..., q_0 - 1, ..., q - 1\}$, in strong and weak regions, respectively. The number of states with energy $E(\boldsymbol{\xi}, \boldsymbol{\eta}, p) = -\frac{1}{2} N \sum_i (p\xi_i + (1 - p)\eta_i)^2$ is

$$\Omega(\boldsymbol{\xi}, \boldsymbol{\eta}, p) = \binom{pN}{pN\xi_0, ..., pN\xi_{q-1}} \binom{(1 - p)N}{(1 - p)N\eta_0, ..., (1 - p)N\eta_{q-1}} \; . \tag{11}$$

- Introducing the Lagrange multipliers a, b, the free energy per site reads

$$\beta f = \sum_i \left(p\xi_i \ln \xi_i + (1 - p)\eta_i \ln \eta_i - \frac{1}{2}\beta (p\xi_i + (1 - p)\eta_i)^2 \right) + a \Big(\sum_i \xi_i - 1 \Big) + b \Big(\sum_i \eta_i - 1 \Big) \; . \tag{12}$$

- The quantities $\boldsymbol{\xi}, \boldsymbol{\eta}$ can take the form

$$\xi_j = \begin{cases} \frac{1}{q_0} (1 + (q_0 - 1) m_0) & , j = 0 \\ \frac{1}{q_0} (1 - m_0) & , j = 1, ..., q_0 - 1 \\ 0 & , j = q_0, ..., q - 1 \; , \end{cases} \tag{13}$$

The HP mean field model

$$\eta_j = \begin{cases} \frac{1}{q} (1 + (q_0 - 1) m_0)(1 + (q/q_0 - 1) m_1) & , j = 0 \\ \frac{1}{q} (1 - m_0)(1 + (q/q_0 - 1) m_1) & , j = 1, ..., q_0 - 1 \\ \frac{1}{q} (1 - m_1) & , j = q_0, ..., q - 1 \; , \end{cases} \tag{14}$$

where m_0, m_1 are the components of a two-fold magnetization $\boldsymbol{m}$.

- Continuous transition: the magnetization at the critical point, $\boldsymbol{m}^*$, must satisfy $\nabla f = (g_0, g_1) = 0$ (it can be shown that $g_0 = 0$ at $m_0^* = 0$). The critical temperature is obtained by the further condition that the Hessian matrix $H(\boldsymbol{m}, \beta, p, q)$ computed at $\boldsymbol{m}^*$ satisfying $m_0^* = 0, \; g_1(\boldsymbol{m}^*, \beta_c, p, q) = 0$, obeys

$$\det H(\boldsymbol{m}^*(\beta_c, p, q), \beta_c, p, q) = 0 \; . \tag{15}$$

- Eq. (15) implicitly determines the second order critical line (for q fixed) in *concentration-temperature* parameter space

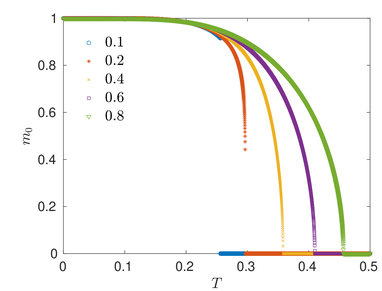
$$\frac{1}{2} \exp \left(\frac{\beta_c - q}{q - 2} \right) = \frac{\beta_c - 2}{(q - 2)(2 - \beta_c p)} \; . \tag{16}$$

- The critical magnetization reads

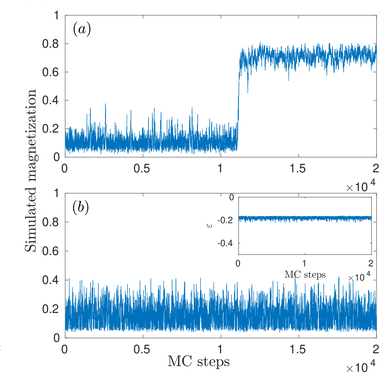
$$\boldsymbol{m}^* = \left(0, \frac{q(2 - \beta_c p)}{\beta_c (1 - p)(q - 2)} - \frac{2}{q - 2} \right) \; . \tag{17}$$

- The critical energy is given by

$$\varepsilon_c = -\frac{(\beta_c - 4)\beta_c + 2q}{2\beta_c^2 (q - 2)} \; . \tag{18}$$



(a) "Strong" magnetization component m_0 as a function of temperature, for different concentrations. It should be noted that the symbols composing the graphs for $p \geq 0.4$ are more dense than for $p \leq 0.2$, in some neighborhood of T_0, where T_0 is the point where the numerical derivative $\frac{\Delta m_0}{\Delta T}$ is "large" .



(b) Magnetization versus MC time for a system with $N = 1000$ spins. (a) $p = 0.1$ and $T = 0.2661$. (b) $p = 0.6$ and $T = 0.4199$ ($T_c = \beta_c^{-1} = 0.409(8)$ according to (16)). Energy, ε, against MC time is plotted in the inset. The energy fluctuates around $\langle \varepsilon \rangle = -0.178(9)$ (c.f. $\varepsilon_c = -0.172(0)$ due to (18).

Figure 2. Analytical and simulated quantities for the MF HP model with spin numbers $q_0 = 2, \; q = 6$. (a) Magnetization component m_0 minimizing (12) and (b) observables (Simulated magnetization $= p^{\frac{q_0 z_0 - 1}{q_0 - 1}} + (1 - p)^{\frac{qz - 1}{q - 1}}$ where z_0 and z are the maximal fractions of monochromatic spins in strong and weak locations, respectively) computed using the Metropolis method.

References

[1] Nir Schreiber, Reuven Cohen, Simi Haber, Gideon Amir, and Baruch Barzel. Unusual changeover in the transition nature of local-interaction potts models. *Physical Review E*, 100(5), November 2019.

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