Self-sustained Clusters in Spin Models and their Link to Ergodicity Breaking

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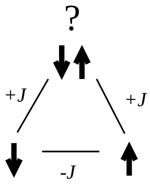
Outline

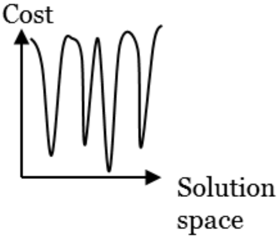
- Background and motivation
- Self-sustained clusters - what does it mean?
- Ising model (Curie-Weiss)
  - Model
  - Entropy of self-sustained clusters
  - Phase transition
- Sherrington-Kirkpatrick model
  - Model - phase diagram
  - Self-sustained clusters in the various phases
- Sparse graphs
  - Ising ferromagnetic model
  - Spin glass and paramagnetic phases
- Summary and future work

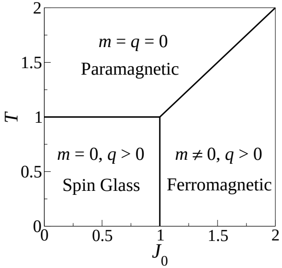
Spin models and hard computational problems

- Spin models - N interacting binary variables
- Disordered systems - fixed sampled interactions/topology
  - Sherrington-Kirkpatrick model - densely connected
  - Viana-Bray model - sparsely connected
  - Hard computational problems (K-SAT, graph colouring)
  - Decoding in error-correcting codes
- Observation - fragmented multi-minima solution spaces
- Optimisation/solution - difficult in some parameter regimes



Frustration





Ergodicity breaking and hard computational problems

Definitions and terminology

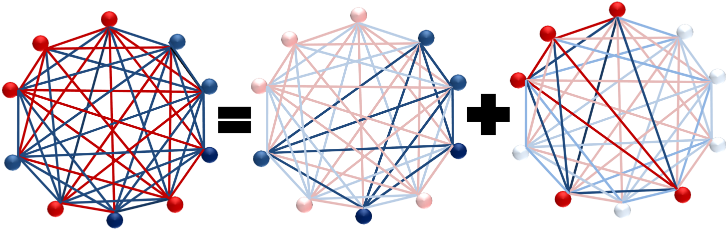
- Ergodicity / ergodicity breaking -
  - *Mathematics:* Ergodicity - same time-averaged behavior as average over the space of all states (phase space); ergodicity breaking - diminishing probability to reach parts of phase space
  - *Physics:* Ergodicity - time spent in a region of the phase space of the same energy is proportional to its volume; typical manifestation of ergodicity breaking - exponential barriers in energy landscape
- Spin/variable space -N spin variables $\mathbf{s}$
- Phase space - separation of space to sets of vectors that share macroscopic properties that constitute a phase
- Solution space - set of vectors $\mathbf{s}$ that obey the constraints (especially at zero temperature)

Self-sustained clusters

Aim: understand the formation of self-sustained clusters and relate them to ergodicity breaking and phase properties

What constitutes a self-sustained clusters $\mathcal{C}$?

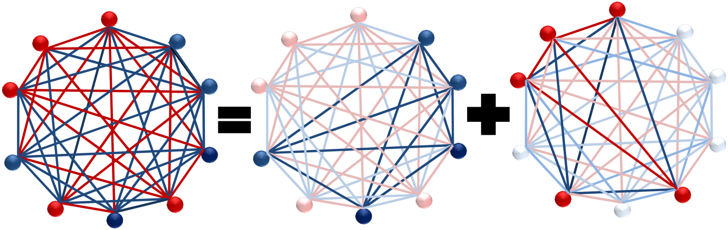
- Denote *in-cluster* ($i \in \mathcal{C}$) and *out-cluster* ($i \notin \mathcal{C}$) spins
- Corresponding magnetic fields $u_i = \sum_{j\in\mathcal{C}} J_{ij}s_j$ and $v_i = \sum_{j\notin\mathcal{C}} J_{ij}s_j$
- Total field - $h_i = u_i + v_i$
- *Self-sustained cluster* if $|u_i| > |v_i|, \ \forall i \in \mathcal{C}$



Self-sustained clusters - interpretation

What does it mean?

- In-cluster variables dominate the state of spins ($i \in \mathcal{C}$)
- $O(1)$ fluctuations do not change state of in-cluster spins
- Macroscopic changes are required to destabilise self-sustained clusters



Models investigated

Sherrington-Kirkpatrick model

- N spin binary variables
- Ferromagnetic ($J_{ij} > 0$) or anti-ferromagnetic ($J_{ij} < 0$) symmetric interactions, randomly drawn from a Gaussian distribution $\mathcal{N}(J_0/N, J^2/N)$; we use $J = 1$
- Hamiltonian $\mathcal{H}_{\mathrm{SK}} = -\sum_{(ij)} J_{ij} s_i s_j$

Ising model (Curie-Weiss)

- Special case of the SK model with $J = 0$ or $J_0 \gg J$
- Hamiltonian - $\mathcal{H}_{\mathrm{Ising}} = -J_0 \sum_{(ij)} s_i s_j / N$.

Analysis used

Replica method

- Replica method - $\ln \mathcal{Z} = \lim_{n\to 0}(\mathcal{Z}^n - 1)/n$ for averaging over instances to obtain expected physical quantities
- Replacing the average of $\ln \mathcal{Z}$ by that of the *replicated partition function* $\mathcal{Z}^n$; using analytical continuation $n \to 0$
- As $N \to \infty$, for densely connected systems, solutions are described *fully and uniformly* by magnetization and inter-replica spin correlation

$$m_\alpha = \frac{1}{N}\sum_i s_{i\alpha}, \qquad q_{\alpha\beta} = \frac{1}{N}\sum_i s_{i\alpha}s_{i\beta},$$

- Replica symmetry ansatz assumed - simplest *replica-symmetric* $m_\alpha = m$ for all α and $q_{\alpha\beta} = q$ for all $\alpha \neq \beta$

Cluster entropy

What is cluster entropy?

- Entropy of clusters $S(r) = [\ln\Omega(r)]/N$; $\Omega(r)$ is the number of self-sustained clusters of normalised size $r = |\mathcal{C}|/N$
- For Ising model at zero temperature all spins are aligned $\Omega(r) = C^N_{Nr} = N!/[(rN)!(N-rN)!]$ and $S(r) = -r\ln r - (1-r)\ln(1-r)$ for $r > 0.5$ (subsets are also counted); and $\Omega(r) = 0$ and $S(r) = -\infty$ otherwise

Calculating cluster entropy

- New variables $\sigma_i = 1, -1$ identify in/out-cluster variables
- An *indicator function*

$$w(\{\sigma_i\},\{s_i\},\{J_{ij}\}) = \prod_i \left[\frac{1-\sigma_i}{2} + \frac{1+\sigma_i}{2}\Theta\left(u_i^2 - v_i^2\right)\right]$$

where $\Theta(x) = 0/1$ for $x \le 0$ and $x > 0$, respectively

Cluster entropy - Ising model

Operator partition function

- At any temperature T we uniformly sample spin configurations of given magnetisation $m = \sum_i s_i / N$, *as it uniquely defines the model's macroscopic properties*

$$
\begin{aligned}
&\mathcal{Z}_{\text{Ising}}(\gamma, m) \\
&\qquad = \operatorname*{\mathbf{Tr}}_{\{s_i\}} \operatorname*{\mathbf{Tr}}_{\{\sigma_i\}} w(\{\sigma_i\}, \{s_i\}) \delta\left(\frac{\sum_i s_i}{N} - m\right) e^{\gamma \frac{\sum_i (1+\sigma_i)}{2}}
\end{aligned}
$$

- w does not depend on $\{J_{ij}\}$ as they are all identical (J_0)
- The parameter γ plays the role of *pesudo-temperature*
- Computing $\mathcal{Z}$ one obtains $S(\gamma)$ and cluster size $r(\gamma)$

Ising model - results

Ising model - entropy and magnetisation

- Self-sustained cluster entropy

$$S(r) = \begin{cases} 0 & r = 0 \\ -\infty & 0 < r < 0.5 \\ -r \ln r - (1-r)\ln(1-r) & r \geq 0.5 \end{cases},$$

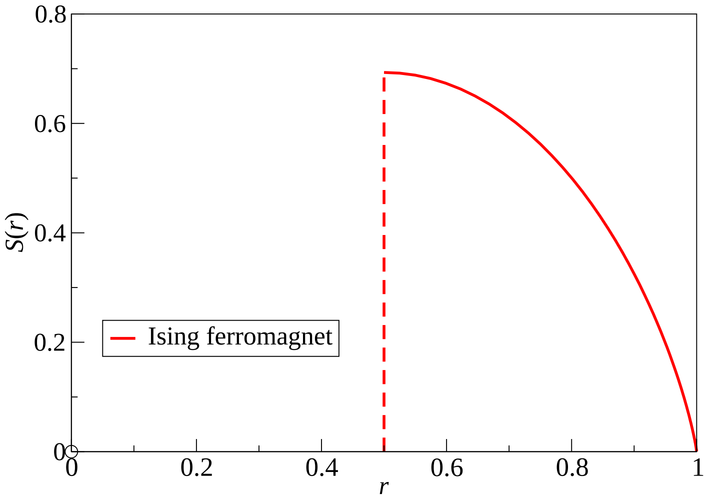
- *In-cluster* and *out-cluster* magnetsations

$$\langle s_i \rangle_{\sigma_i = 1} = \frac{m + m_{s\sigma}}{2r}, \qquad \langle s_i \rangle_{\sigma_i = -1} = \frac{m - m_{s\sigma}}{2(1-r)}$$

where $m = \frac{1}{N} \sum_i s_i$ and $m_{s\sigma} = \frac{1}{N} \sum_i \sigma_i s_i$

- Trivial ergodicity breaking occurs in the ferromagnetic phase due to symmetry with either $m > 0$ or $m < 0$; trivial clusters span the whole system

Ising model - results



Operator partition function

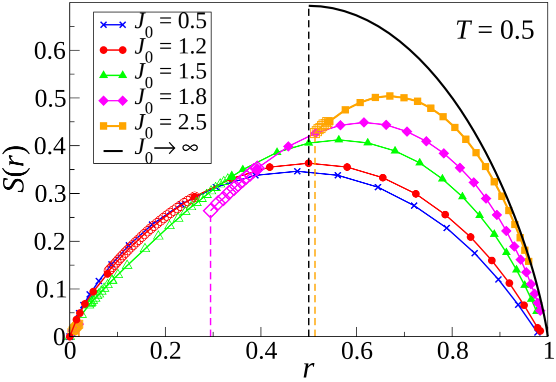
- We uniformly sample spin configurations of given magnetization $\{m_\alpha\}$ and cross-replica overlap $\{q_{\alpha\beta}\}$, *which uniquely define the model's macroscopic properties*
- Replicated operator partition function

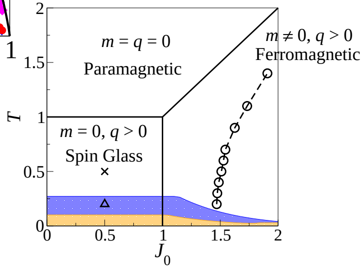
$$\begin{aligned}
&\Xi_{\mathrm{SK}}(\gamma,\{m_\alpha\},\{q_{\alpha\beta}\},n) \\
&= \operatorname*{\mathbf{Tr}}_{\{J_{ij}\}} \operatorname*{\mathbf{Tr}}_{\{s_{i\alpha}\}} \operatorname*{\mathbf{Tr}}_{\{\sigma_{i\alpha}\}} e^{\gamma \sum_{i,\alpha} \frac{1+\sigma_{i\alpha}}{2}} \prod_{\alpha} w(\{\sigma_{i\alpha}\},\{s_{i\alpha}\},\{J_{ij}\}) \\
&\times \prod_{\alpha} \delta\left(\frac{\sum_i s_{i\alpha}}{N} - m_\alpha\right) \prod_{\alpha\beta} \delta\left(\frac{\sum_i s_{i\alpha} s_{i\beta}}{N} - q_{\alpha\beta}\right) \prod_{(ij)} P(J_{ij}).
\end{aligned}$$

Replica symmetry breaking

- Un-replicated partition function $\mathcal{Z}_{\rm SK}[\gamma, P(m_\alpha), P(q_{\alpha\beta})]$ requires averaging over the distributions $P(m_\alpha)$ and $P(q_{\alpha\beta})$ to compute $\ln \mathcal{Z}_{\rm SK} = \lim_{n\to 0}(\Xi_{\rm SK} - 1)/n$
- In the spin glass phase *Full Replica Symmetry Breaking* (FRSB) ansatz is required
- We use Replica Symmetry (and one-step RSB) so that $\ln \mathcal{Z}_{\rm SK}$ only depends on γ, m and q
- RS/1RSB ansatze used in parameter values where the corresponding entropy is positive

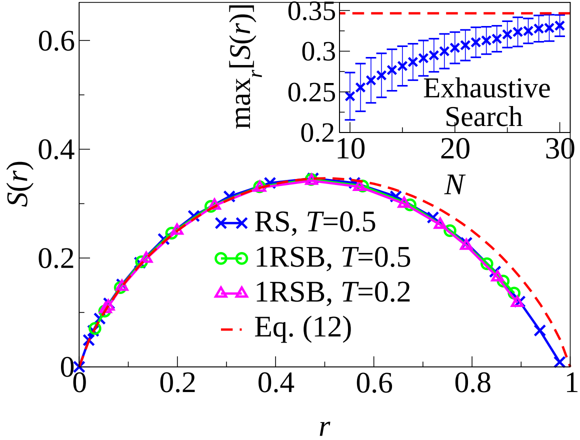
SK model in the ferromagnetic phase





Entropies exhibit a similar general shape but with degrees of freedom reduced (almost exactly) by *half*; and a gap at $r = 1$

$$S(r) \approx \frac{-r\ln r - (1-r)\ln(1-r)}{2} = \lim_{N\to\infty} \frac{\ln C_{Nr/2}^{N/2}}{N}$$



Clusters in the spin-glass phase I

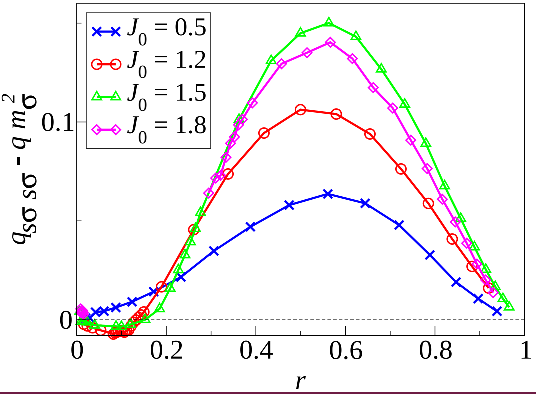
Correlations between clusters and replica

- To understand the relation between self-sustained clusters and ergodicity breaking we examine $d = q_{s\sigma s\sigma} - qm_\sigma^2$

$$q_{s\sigma s\sigma} = [\langle s_{i\alpha}\sigma_{i\alpha}s_{i\beta}\sigma_{i\beta}\rangle_{i,\alpha,\beta}], \quad m_\sigma = [\langle \sigma_{i\alpha}\rangle_{i,\alpha}],$$

  $[\ldots]$ denotes disorder average
- If spin-configuration overlap between two replica is uncorrelated with cluster affiliations $d = 0$
- When correlated spin-configurations in two replica have correlated cluster associations $d > 0$

Clusters in the spin-glass phase II

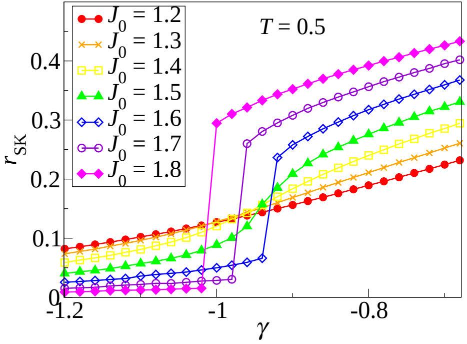


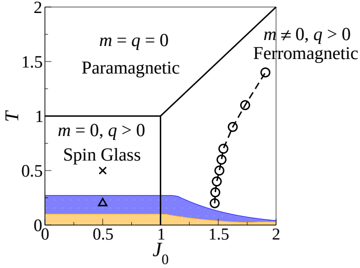
Correlations between clusters and replica - results

- $d > 0$ for all r - correlated *self-sustained* and *frozen* clusters of all sizes; not all spin subsets are self-sustained clusters ($d = 0$)
- An extensive number of spin flips are required to macroscopically destabilise self-sustained clusters

Ferromagnetic phase - gap in cluster sizes

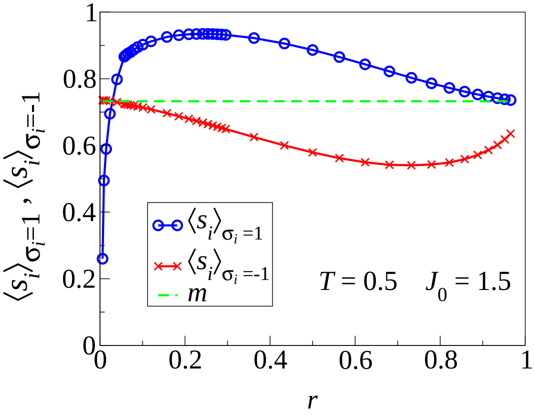
- Discontinuity in cluster size at $J_0 \geq 1.6$; division to large/small clusters; small domains of arbitrary alignment always exist
- Phase line marks a growing ferromagnetic domain with J_0 - leading to trivial cluster as $J_0 \to \infty$





Cluster sizes and magnetisations

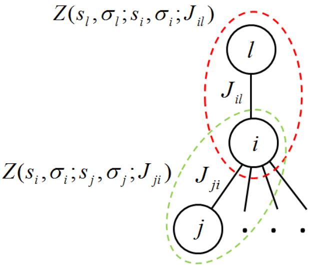
- In-cluster magnetisation as a function of r - imbalance between different clusters $\langle s_i \rangle_{\sigma_i=1} > m$ and $\langle s_i \rangle_{\sigma_i=-1} < m$
- Pointing to local domains of weaker magnetic alignment
- Absent in the Ising ferromagnet; a feature of coupling disorder



Recursion relation in sparse graphs

- For sparse graphs, we write down a recursion to relate the operator partition function of node i to descendent nodes j's:

$$\mathcal{Z}(s_l,\sigma_l;s_i,\sigma_i;J_{il}) \propto \underset{\{s_j,\sigma_j\}}{\mathbf{Tr}}\, w\left(s_i,s_l,\{s_j\};\sigma_i,\sigma_l,\{\sigma_j\};J_{il},\{J_{ji}\}\right)$$
$$\times\, e^{\gamma\frac{1+\sigma_i}{2}}\left[\prod_{j=1}^{k_i-1}\mathcal{Z}(s_i,\sigma_i;s_j,\sigma_j;J_{ji})\right]P(s_i)P(J_{il})$$



The indicator function

$$w\left(s_i,s_l,\{s_j\};\sigma_i,\sigma_l,\{\sigma_j\};J_{il},\{J_{ji}\}\right)$$
$$=\left[\frac{1-\sigma_i}{2}+\frac{1+\sigma_i}{2}\Theta(u_i^2-v_i^2)\right]$$

is defined similarly as in the fully connected cases

Self-sustained clusters on sparse graphs II

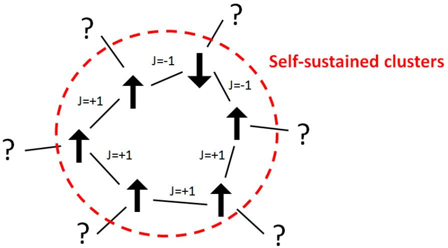
Recursion relation in sparse graphs (cont.)

- The spin configuration is uniformly sampled from the order parameter $P(s_i)$, obtained from a self-consistent equation independent of σ's:

$$P(s_i) = \underset{\{s_j\}}{\mathbf{Tr}}\, e^{\beta \sum_{j=1}^{k_i-1} J_{ji} s_j s_i} \prod_{j=1}^{k_i-1} P(s_j)$$

and simplifies to a recursion of cavity field h_i by $P(s_i) \propto e^{\beta h_i s_i}$

- Loops in 3-regular graphs form self-sustained clusters at low temperature
- Reason for frustrations or RSB?



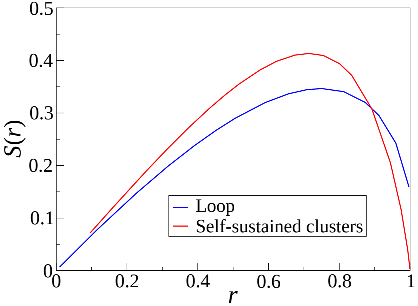
The Ising model on random graphs

A simple case

- The Ising model on random graphs can be constructed by setting all $J_{ij} = 1$
- At $T = 0$, all $s_i = 1$ (or -1), the recursion of the operator partition function can be greatly simplified:

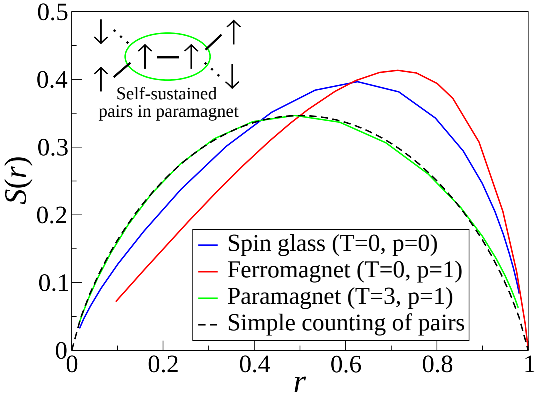
$$\mathcal{Z}(\sigma_l, \sigma_i) \propto \operatorname*{\mathbf{Tr}}_{\{\sigma_j\}} w\left(\sigma_i, \sigma_l, \{\sigma_j\}\right) e^{\gamma \frac{1+\sigma_i}{2}} \prod_{j=1}^{k_i - 1} \mathcal{Z}(\sigma_i, \sigma_j)$$

- Random regular network of $k = 3$, all $J = 1$ at $T = 0$:
- More cluster than loop at most size r, since clusters are not necesarily loop only
- Less cluster then loop at $r = 1$, since more than one loop span the network



Model and cluster entropy

- The distribution of coupling is given by $P(J_{ij}) = p\delta(J_{ij}-1) + (1-p)\delta(J_{ij}+1)$
- The three main phases on 3-regular graphs: ferromagnetic, paramagnetic and spin glass phase



Summary and future work

Summary

- Defined the notion of self-sustained clusters
- Developed a method to calculate the entropy of self-sustained clusters; obtained results for fully and sparsely connected Ising models, SK model and spin glasses on random graphs
- Showed that their existence is correlated with ergodicity breaking in the examples studied; due to system symmetries or complexity of the energy landscape
- Identified a new phase transition in the ferromagnetic regime

Future plan

- Explore further properties of self-sustained clusters in sparsely connected networks
- Improve optimisation algorithms using the new insight gained

C-H. Yeung, D. Saad, *Phys. Rev. E* **88**, 032132 (2013)