Ultrametricity and clustering of states in spin glasses

A one-dimensional view

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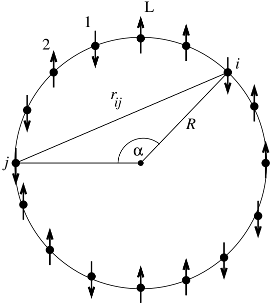
Outline

- 1d model with variable dimension
- Ultrametricity
- Hierarchical clustering

1-dimensional long-range spin glass

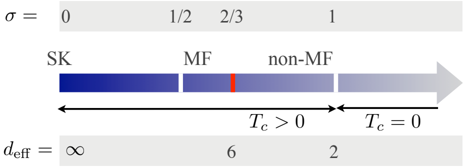
N Ising spins $S_i = \pm 1$ on a ring
tunable long-range interaction

$$\mathcal{H} = -\sum_{i<j} J_{ij} S_i S_j \,, \quad J_{ij} = c(\sigma) \frac{\epsilon_{ij}}{{r_{ij}}^{\sigma}}$$



ϵ_{ij} quenched Gaussian $N(0,1)$
$c(\sigma)$ such that $1 \overset{!}{=} T_{\mathrm{c}}^{MF}[c(\sigma)]$
[Kotilar/Anderson/Stein, PRB 1983]

Phase diagram:



close to $\sigma = 2/3$:
$d_{\mathrm{eff}} \approx 2/(2\sigma - 1)$
[Bhatt/Young, JMMM 1986]

Nature of the spin-glass phase

Mean-Field Picture

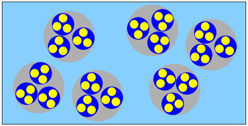
$\sigma < 1/2$

$\longleftrightarrow$

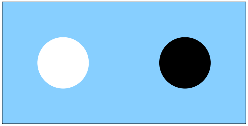
Droplet Picture

$\sigma > 1$

There are MANY states



There are TWO states



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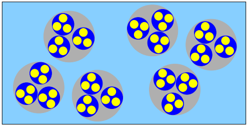

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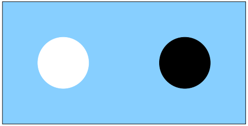
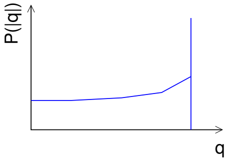
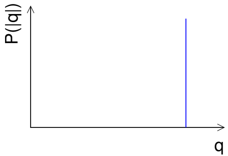




overlaps:

$$q_{\alpha\beta} = \frac{1}{N}\sum_i S_i^{\alpha} S_i^{\beta}$$



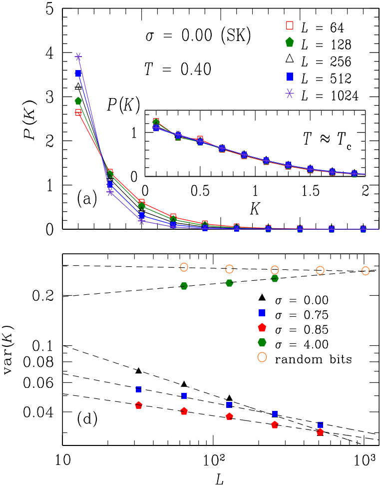
Ultrametricity

Distance $d_{\alpha\beta} = 1 - |q_{\alpha\beta}| \rightarrow$ respects spin-flip symmetry

Ultrametricity (proven $\sigma = 0$):
$d_{\alpha\beta} \leq \max\{d_{\alpha\gamma}, d_{\gamma\beta}\}$
$\rightarrow \quad d_{\max} \geq d_{\mathrm{med}} \geq d_{\min}$
$\Rightarrow \quad d_{\max} = d_{\mathrm{med}}$
$\rightarrow \quad K = (d_{\max} - d_{\mathrm{med}})$:
$P(K) \rightarrow \delta(K)$ for $N \rightarrow \infty$

But: Random bits ($N \rightarrow \infty$):
$d_{\max} = d_{\mathrm{med}} = d_{\min}$

$\rightarrow \quad K = (d_{\max} - d_{\mathrm{med}})/\rho$
(ρ width of d distribution)



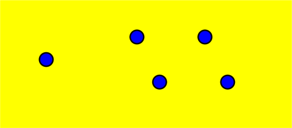
Numerics: Parallel Tempering Monte Carlo $T \in [0.4T_c, 1.4T_c]$

[H.G. Katzgraber and AKH, arXiv:0807.3513]

Hierarchical Clustering

- Start: Z configs $= Z$ single configuration clusters $C_\alpha = \{\underline{S}^\alpha\}$ initial distances $\tilde{d}(C_\alpha, C_\beta) = d_{\alpha\beta}$
- Merge iteratively nearest clusters $C_{\text{new}} = C_\alpha \cup C_\beta$, update $\tilde{d}(C_{\text{new}}, C_\gamma) = \ldots\ (\gamma \neq \alpha, \beta)$, until one cluster left.

  [J.H. Ward, J. Am. Stat. Assoc. 1963]



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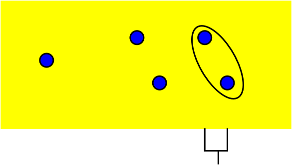

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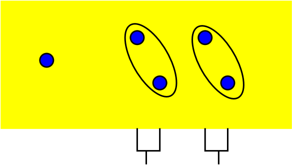

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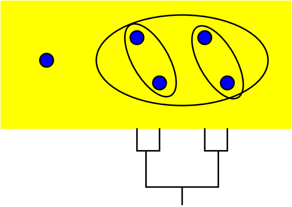

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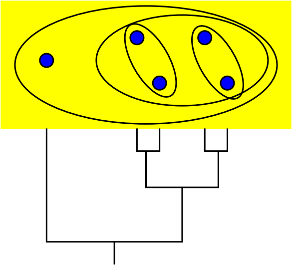
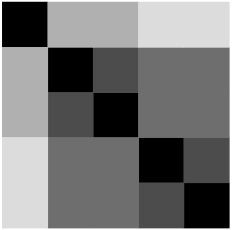


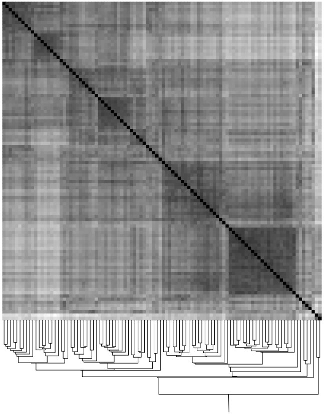
$d(\underline{S}^\alpha, \underline{S}^\beta)$:



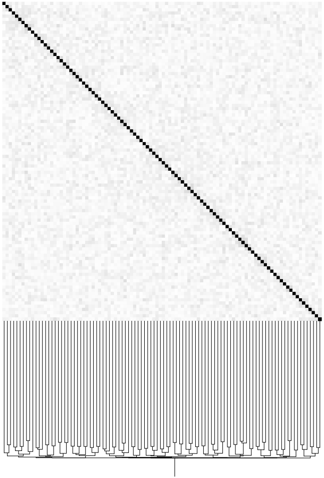
Sample results

SK model ($\sigma = 0.0$), $L = 1024$, 100 configurations

$T = 0.4$



$T = 1.4$



(distance of horizontal line from matrix $\leftrightarrow$ distance of clusters whe merged)

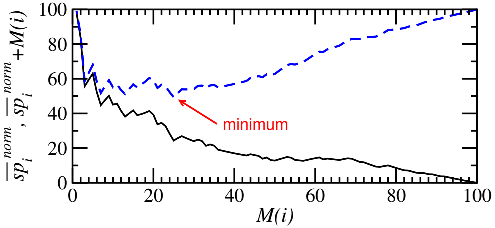
Number of clusters

- During clustering at step i: $M(i) = M - i$ clusters $\{C_\gamma\}$
- For each cluster C:

spread $$sp_C = \frac{2}{|C|(|C|-1)} \sum_{\alpha \neq \beta \in C} d_{\alpha\beta}$$

[Kelley/Gardner/Sutcliffe, Prot.Eng.1996]

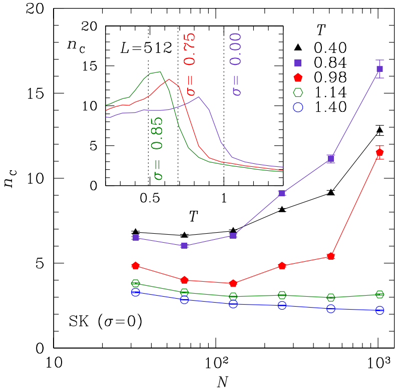
→ averaged + normalized spread $\overline{sp}_i^{\text{norm}} \in [1, M-2]$



- $P_i := \overline{sp}_i^{\text{norm}} + \gamma M(i)$ (γ= "sensitivity")
  - $\overline{sp}_i^{\text{norm}}$ small, if clusters compact
  - $M(i)$ small, if few clusters

→ $I_{\min} = \operatorname{argmin}_i \{P_i\}$, $c = M(i_{\min})$ = number of clusters

- For each system size N:
  For 100 realizations of set of M random strings ($T = \infty$):
  Choose γ such that $\overline{c} = c_0 = 1.1$
- Results:



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- Result depends on c_0: peak moves left for decreasing c_0

Summary

- 1d long-range model:
  tunable from mean-field to simple behavior
- Normalize "degree of ultrametricity" by
  width of distance distribution
  $\rightarrow$ Exhibits ultrametricity close to $\sigma = 1$ ($d_{\mathrm{eff}} = 2$)
- Determine clusters via "spread" of configurations
  $\rightarrow$ Cluster numerically "visible" close to $\sigma = 1$.