New insights from one-dimensional spin glasses

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Outline and Motivation

- Introduction to spin glasses (disordered magnets)
  - What are spin glasses?
  - Why are they hard to study?

- How well does the mean-field solution work?
  - Model: 1D chain
  - Do spin glasses order in a field?
  - Ultrametricity in spin glasses?

- Applications to other problems and algorithm benchmarking.

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- Applications to other problems and algorithm benchmarking.
Brief introduction to spin glasses
Building a spin glass from the Ising model

- **Hamiltonian:**
  \[
  \mathcal{H} = - \sum_{\langle ij \rangle} J_{ij} S_i S_j - H \sum_i S_i
  \]
  \[
  J_{ij} = 1 \quad \forall i, j \quad i \neq j
  \]

- **Order parameter:**
  \[
  m = \frac{1}{N} \sum_i S_i \quad \text{(magnetization)}
  \]

- **Some properties:**
  - Phase transition to an ordered state.
  - According to Harris criterion, if \( d\nu > 2 \) the system changes universality class when local disorder is added.
  - For the Ising model \( d\nu \leq 2 \) in 2D and 3D.
What is a spin glass?

- **Prototype model**: Edwards-Anderson Ising spin glass

\[ \mathcal{H} = -\sum_{ij} J_{ij} S_i S_j - h \sum S_i \quad J_{ij} \text{ random} \]

- **Properties**:
  - Phase transition into a glassy phase
  - Complex energy landscape
  - Some hallmarks: aging, memory, hysteresis, ...
  - Complex optimization problem
  - Very hard to treat analytically beyond mean-field.
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Many applications to other problems!
Applications beyond disordered magnets

- The models can describe many systems with competing interactions on a graph:
  - **Computer chips:**
    
    \[ S_i \] component
    
    \[ J_{ij} \] wiring diagram
  - **Economic markets:**
    
    \[ S_i \] agent inclination
    
    \[ J_{ij} \] portfolio interactions
  - **Other applications:**
    
    - Quantum error correction in topological quantum computing (current research).
    - Optimization problems (e.g., number partitioning problem).
    - Neural networks, …
Early experimental observations:
- 1970: Canella and Mydosh see a cusp in the susceptibility of Fe/Au alloys (disorder). Material with RKKY interactions (frustration):

\[
J_{ij} \sim \frac{\cos(2k_F R_{ij})}{R_{ij}^3}
\]

Early theoretical descriptions:
  \[
  \mathcal{H} = - \sum_{\langle ij \rangle} J_{ij} S_i S_j \quad \text{mean-field approx.} \quad \sum_{\langle ij \rangle} \to \sum_{i,j}
  \]
- 1975: Mean-field Sherrington-Kirkpatrick model.
- 1979: Parisi solution of the mean-field model (RSB).
- 1986: Fisher, Huse, Bray, Moore introduce the phenomenological droplet picture (DP) for short-range systems.
How can we study these systems?

- **Analytically:** only the mean-field solution (RSB) or qualitative descriptions (DP).

- **Numerically:** Optimal problem for large computers
  - Challenges:
    - Exponential number of competing states (usually NP hard).
    - Relaxation times diverge exponentially with the system size.
    - Extra overhead due to disorder averaging.
    - Usually small systems only.
  - Solution:
    - Use large computer clusters.
    - Use better algorithms.
    - Use better models.
  - Average project requires 300’000 CPUh (4 months on $10^2$ CPUs).
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Some open problems... many challenges

Some open issues:
- Chaos in spin glasses
- Nature of the low-temperature spin-glass phase
- Properties of vector spin glasses, ...

And many more:
- ultrametricity
- universality
- memory effect
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And many more:
- Which properties of the mean-field solution carry over to short-range systems?
Models: The 1D Ising chain
Traditional model: Edwards-Anderson

- **Hamiltonian:**
  \[ H = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j \quad S_i \in \{\pm 1\} \]

- **Details about the model:**
  - Nearest-neighbor interactions.
  - Simulations usually done with periodic boundary conditions.
  - Transition temperatures: \( T_c = 0 \) (2D), \( T_c \sim 1 \) (3D), \( T_c \sim 2 \) (4D).
  - Most studied spin-glass model to date.

- **Disadvantages of the model:**
  - Cannot be solved analytically.
  - In high space dimensions only small systems can be simulated \((D \geq 5\) almost impossible).
Better: The one-dimensional Ising chain

\[ \mathcal{H} = - \sum_{ij} J_{ij} S_i S_j - \sum_i h_i S_i \]

- **Properties:**
  - The sum ranges over all spins
  - Power-law random interactions

\[ J_{ij} \sim \frac{\varepsilon_{ij}}{r_{ij}^{\sigma}} \]

- **Advantages:**
  - Large range of sizes.
  - Tuning the power-law exponent changes the universality class.

Fisher & Huse, PRB (88)
Kotliar et al., PRB (83)
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- \( T_c > 0 \)
- \( \sigma_{c(d)} \)
- \( d = 2\sigma \)
- \( d = \sigma \)

---

Fisher & Huse, PRB (88)
Kotliar et al., PRB (83)
Tuning the universality class

- Short-range spin glasses:
  - Upper critical dimension $d_u = 6$ (for $d \geq d_u$ MF behavior)
  - Lower critical dimension $d_l = 2$ (for $d \leq d_l$ $T_c = 0$)

- Phase diagram of the 1D chain:

\[ d_{\text{eff}} \approx \frac{2}{2\sigma - 1} \]

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- Phase diagram of the 1D chain:

<table>
<thead>
<tr>
<th>$\sigma$</th>
<th>0</th>
<th>1/2</th>
<th>2/3</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>SK</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MF</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>non-MF</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$T_c > 0$ $T_c = 0$

$d_{\text{eff}} = \infty$ 6 2

expect MF predictions to work

Kotliar et al., PRB (83)
Algorithms
Reminder: Exchange Monte Carlo

- Efficient algorithm to treat spin glasses at finite $T$.
- Idea:
  - Simulate $M$ copies of the system at different temperatures with $T_{\text{max}} > T_c$ (typically $T_{\text{max}} \sim 2T_c^{\text{MF}}$).
  - Allow swapping of neighboring temperatures: easy crossing of barriers.

- Extremely fast equilibration at low temperatures.
- For the following applications we use this algorithm...

Hukushima & Nemoto (96)
Do spin glasses order in a field?
Spin-glass state in a field?

- Two possible scenarios:
  - Replica Symmetry Breaking (RSB): existence of an instability line [Almeida & Thouless (78)] for the mean-field SK model.
  - Droplet picture (DP): there is no spin-glass state in a field.

Why should we care?

- The question lies at the core of theoretical descriptions.
- Field terms are ubiquitous in applications/experiments.
- Experimentally, numerically, and theoretically controversial.
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Probing criticality: correlation length

• Use the finite-size correlation length to probe criticality in spin-glass systems:

  • Wave-vector-dependent connected spin-glass susceptibility:
    \[ \chi_{SG}(k) = \frac{1}{N} \sum_{ij} \left[ \left( \langle S_i S_j \rangle_T - \langle S_i \rangle_T \langle S_j \rangle_T \right)^2 \right] \text{dis} \]
    \[ e^{ik(R_i - R_j)} \]

  • Perform an Ornstein-Zernicke approximation:
    \[ \frac{\chi_{SG}(k)}{\chi_{SG}(0)}^{-1} = 1 + \xi_L^2 k^2 + O[(\xi_L k)^4] \]

  • Compensate for finite-size effects and periodic boundaries:
    \[ \xi_L = \frac{1}{2 \sin(k_{\text{min}}/2)} \left[ \frac{\chi_{SG}(0)}{\chi_{SG}(k_{\text{min}})} - 1 \right]^{1/2} \]

    • Finite-size scaling:
      \[ \frac{\xi_L}{L} = \tilde{X} \left( L^{1/\nu} [T - T_c] \right) \]

    • Better than Binder ratio.
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Ballesteros et al. PRB (00)
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How well does this work for zero field?

- Study the 3D model:
  \[ H = - \sum_{\langle i,j \rangle} J_{ij} S_i S_j \]

- Remember:
  \[ \frac{\xi_L}{L} = \tilde{\xi} [L^{1/\nu}(T - T_c)] \]

- The data cross at \( T_c \approx 0.96 \).

- Spin-glass state at zero field.

- Next: apply a field…

Katzgraber et al., PRB (06)
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Katzgraber et al., PRB (06)
“Old” 3D results in a field

- Perform “slices” at different horizontal fields.

\[ \mathcal{H} \rightarrow \mathcal{H} - \sum_{i} h_i S_i \]

\( H = 0.3 \)

Katzgraber & Young, PRL (04)
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\[ T \]

\[ T_c \]

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Problem: small systems.

Maybe AT line for $d \geq d_u$?

$H = 0.05$ Does the method pick up the AT line?

No AT line in 3D.

$H = 0.05$ $\sum_i h_i S_i$

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- Solution: Use 1D chain
  - Can probe large systems.
  - Can probe MF region to check if the method works.

Katzgraber & Young, PRL (04)

\[ H = 0.05 \]

Does the method pick up the AT line?

No AT line in 3D.
Tuning the universality class (1D chain)

- External field $H = 0.10$.
- The data span a large range of system sizes.
- The AT line vanishes outside the MF regime ($\sigma \geq 2/3$).

![Diagram showing AT line and critical exponents](Image)

Katzgraber & Young, PRB (2005)
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![Graph showing $\xi_L/L$ vs. $T$ with different $\sigma$ values and system sizes.](image)

$\sigma = 0.75$

Katzgraber & Young, PRB (2005)
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Katzgraber & Young, PRB (2005)
Spin-glass state in a field?

- The AT line vanishes when not in the mean-field regime.
- For short-range spin glasses below the upper critical dimension:

$$H_{AT}$$

Does the behavior change for even larger system sizes?
- What happens for “narrow” AT lines? (see cond-mat/0712.2009)
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Ultrametricity in spin glasses
What is ultrametricity?

• Formal definition:
  • Given a metric space with a distance function.
  • In general, the distance function obeys the triangle inequality:
    \[ d(\alpha, \gamma) \leq d(\alpha, \beta) + d(\beta, \gamma) \]
  • In an ultrametric space we have a stronger inequality:
    \[ d(\alpha, \gamma) \leq \max\{d(\alpha, \beta), d(\beta, \gamma)\} \]

• Note:
  • Every triangle is isosceles in an ultrametric space.

• Examples:
  • Linguistics (space where words differ)
  • Taxonomy (classification of species).
  • Number theory (p-adic numbers), ...
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Relevance to spin glasses (hand-waving…)

- Replica symmetry breaking solution of the mean-field model:
  \[ F = -kT[\log Z]_{av} \quad \text{and} \quad \log Z = \lim_{n \to 0} \left( \frac{Z^n - 1}{n} \right) \]

- Order parameter: overlap function
  \[ q = \frac{1}{N} \sum_{i=1}^{N} S_i^\alpha S_i^\beta \]
  \[ q = \frac{1}{N} \alpha \times \beta \]

- After replication one obtains:
  \[ [\log Z]_{av} \sim \int \Pi_{\alpha, \beta} dQ_{\alpha\beta} e^{NG(Q_{\alpha\beta})} \]

- Typical structure:
  \[ Q_{\alpha\beta} = \frac{1}{N} \sum_{i=1}^{N} S_i^{(\alpha)} S_i^{(\beta)} = \]

- One can show that for three states in \( Q_{\alpha\beta} \) with \( q_{\alpha\gamma} \geq q_{\gamma\beta} \geq q_{\alpha\beta} \)
  one has \( q_{\gamma\beta} = q_{\alpha\beta} \) in the thermodynamic limit.

Parisi (79)
Talagrand (06)
What does it mean to be ultrametric?

- Simple test to see if the mean-field solution is applicable to a model:
  - Ultrametricity is a cornerstone of the mean-field solution.
  - If a model has no ultrametricity, the RSB solution is not valid for it.

- Current state of affairs:
  - Are short-range models ultrametric? Very controversial!
  - Many contradicting predictions.

- Problems:
  - Only small short-range systems can be studied.
  - The states for the test have to be selected very carefully.

- Solution:
  - Analysis of the 1D chain [similar to Hed et al. (04)].

Hed et al., PRL (04)
Contucci et al., PRL (06)
Jörg & Krzakala, PRL (07)
and many more...
Achtung! Problems when picking 3 states…

Possible pitfalls:

1. If time-reversal symmetry is unbroken, one has to ensure that all three states used belong to the same “side” of phase space.
2. The temperature must be much smaller than $T_c$.
3. If the temperature is too small, for large systems most triangles are equilateral (carry no information). Do not study too low $T$’s.

Solutions:

1. Can be avoided with a clustering analysis: Pick 3 states only from the left tree.
2. Simulations done at $T < T_c$, but not below $T = 0.2T_c$. Data shown for $T = 0.4T_c$.
3. To avoid equilateral triangles pick the 3 states from different branches in the left subtree ($C_{1a}$, $C_{1b}$, $C_2$). Next…
Selection of states (similar to Hed et al.)

- **Generation of states:**
  - Equilibrate system.
  - Store $10^3$ states per realization.

- **Selection of states:**
  - Sorted *dendrograms* using Wards clustering method.
  - Pick left tree (“spin down”).
  - Split left tree into $|C_1| \geq |C_2|$.
  - Split $C_1$ into $C_{1a}$ and $C_{1b}$.
  - Pick three random states: $\alpha \in C_{1a}, \beta \in C_{1b}, \gamma \in C_2$.

- **Distance matrix:**
  - Darker colors mean closer distances $d_{\alpha\beta} = (1 - q_{\alpha\beta})/2$. 

---

2.

from Hed et al., PRL (04)
Typical distance matrices at $T < T_c$

- Data for the 1D chain, $L = 512, T = 0.4T_c$.

Darker colors correspond to closer hamming distances.
- Both systems show structure at low temperatures.
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How to measure ultrametricity

- **Observable:**
  - Select three states with the aforementioned recipe.
  - Compute the hamming distance between them: \( d_{\alpha\beta} = (1 - q_{\alpha\beta})/2 \).
  - Sort the distances: \( d_{\text{max}} \geq d_{\text{med}} \geq d_{\text{min}} \).
  - Compute:
    \[
    K = \frac{d_{\text{max}} - d_{\text{med}}}{\rho(d)}
    \]
    
    Here \( \rho(d) \) is the width of the distance distribution.

- **Signs of ultrametricity:**
  - If the space is ultrametric, we expect \( d_{\text{max}} = d_{\text{med}} \) for \( N \to \infty \).
  - Study the distribution \( P(K) \). We expect:
    \[
    P(K) \sim \delta(K = 0) \quad N \to \infty
    \]
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    K = \frac{d_{\text{max}} - d_{\text{med}}}{\rho(d)}
    \]
    Here $\rho(d)$ is the width of the distance distribution.

- Signs of ultrametricity:
  - If the space is ultrametric, we expect $d_{\text{max}} = d_{\text{med}}$ for $N \to \infty$.
  - Study the distribution $P(K)$. We expect:
    \[
    P(K) \sim \delta(K = 0) \quad N \to \infty
    \]
Distributions $P(K)$ at $T = 0.4T_c$

Currently: try to determine the number of RSB layers and clusters.

Similar results for other values of $\sigma$. 

Katzgraber & Hartmann, submitted

$\sigma = 0.75$
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indication of ultrametricity?
What else can we do with the 1D chain?
Other ideas currently explored

- Study open problems in spin glasses:
  - Chaos, aging, universality, memory effect, …

- Modifications of the model:
  - Spin symmetries (Potts, Heisenberg, …).
  - $p$-spin model for structural glasses.
  - Power-law probability-diluted chain (huge systems).

- Benchmarking algorithms:
  - How does the algorithm scale with the size of the input ($N$)?
  - How does the scaling of the algorithm depend on the complexity/connectivity?
  - 1D chain: range of the interactions (universality class) can be changed.
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*Matsuda et al. (07)*

![Graph showing critical temperatures $T_c$, $T_w$, and $T$ with $\chi_{AC}$ as a function of $T$.]
Probability-diluted Gaussian Ising chain

- Place a Gaussian random bond with $P(J_{ij} \neq 0) \sim r^{-2\sigma}$
- Same behavior as the regular 1D chain, but $[z]_{av} = 2\zeta(2\sigma)$.

Note: Leuzzi et al. fix the connectivity (VB limit). Here SK limit.

$H = -\sum_{i<j} J_{ij} S_i S_j$

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now revisiting the AT line…

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\( L \)
Example: Hysteretic optimization

Experiment:
- Do you have a CRT monitor or a non-LCD TV at home?
- Take a magnet and hold it to the screen.
- You are in trouble.

Solution:
- Call the technician.
- Make a degaussing coil and slowly do circles around the TV increasing the radius and distance.

You have just hysteretically (and possibly also hysterically) demagnetized the TV screen.
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Idea: Minimize the energy of a system by successive demagnetization.

Example: Ising spin glass

\[ \mathcal{H} = - \sum_{ij} J_{ij} S_i S_j - H \sum_i \xi_i S_i \]

\[ m = \frac{1}{N} \sum_i \xi_i S_i \]

\[ \xi_i = \pm 1 \text{ random} \]

\[ H_{\text{sat}} \rightarrow \gamma H_{\text{sat}} \]

for details see Hartmann & Rieger book (04)
Benchmarking: Hysteretic optimization

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- The algorithm works best in the **infinite-range** regime.

for details see Hartmann & Rieger book (04)

adapted from Gonçalves & Boettcher (08)

Zarand et al., PRL (02)

\[ H_{\text{sat}} \rightarrow \gamma H_{\text{sat}} \]

\[ E \]

\[ E_0 \rightarrow dH \]

\[ \sigma \]

\[ L \]

\[ \text{64} \quad \text{128} \quad \text{256} \]
Benchmarking: Hysteretic optimization

- Idea: Minimize the energy of a system by successive demagnetization.
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  \[ \mathcal{H} = - \sum_{ij} J_{ij} S_i S_j - H \sum_i \xi_i S_i \]
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  \[ H_{\text{sat}} \rightarrow \gamma H_{\text{sat}} \]

- The algorithm worked in the infinite range regime.

adapted from Gonçalves & Boettcher (08)

Other algorithms tested: PT, hBOA, BCP, ...

for details see Hartmann & Rieger book (04)
New insights from one-dimensional spin glasses
New insights from one-dimensional spin glasses

- **Summary:**
  - Do short-range spin glasses order in a field? No.
  - Are short-range spin glasses ultrametric? Seems like it.
  - What does this mean? The mean-field solution works only for certain aspects.

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  - Large systems can be studied.
  - The effective space dimension can be changed.
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