Studying Spin Glasses via Combinatorial Optimization

Frauke Liers

Emmy Noether Junior Research Group,
Department of Computer Science, University of Cologne

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What we are interested in...

- develop, improve and implement algorithms for optimization problems occuring in physics:
  ground states of
  - Ising spin glasses in different dimensions
  - Potts glasses
  - Potts glasses for $q \to \infty$
  - etc.
- study their physics together with physics colleagues

We always compute exact ground states!
methods we use:

- polynomial algorithms (matching, maximum flow algorithms, etc.)
- branch-and-bound or branch-and-cut algorithms with exponential worst-case running time

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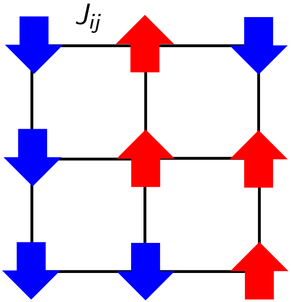
Spin Glasses

e.g. $Rb_2Cu_{1-x}Co_xF_4$
experiments (Cannella & Mydosh 1972) reveal:
at low temperatures: $\rightarrow$ phase transition spin glass state
Edwards Anderson Model (1975)

- short-range model
- interactions randomly chosen
  - $J_{ij} \in \{+1, -1\}$ or
  - Gaussian distributed
- $H(S) = -\sum_{<i,j>} J_{ij} S_i S_j$, with spin variables S_i



ground state: $\min\{H(\underline{S}) \mid \underline{S}$ is spin configuration$\}$

Outline

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1. Hard Ising Spin Glass Instances
2. $2d$ Ising Spin Glasses in a Field
3. Potts Glasses
4. Potts Glasses with $q \longrightarrow \infty$

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'This is a Hard Problem' means...

- NP-hard, i.e. we cannot expect to find an algorithm that solves it in time growing polynomial in the size of the input
- e.g., $2d$ Ising spin glasses with an external field or $3d$ lattices
- whereas $2d$, no field, free boundaries: 'easy'

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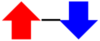
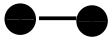
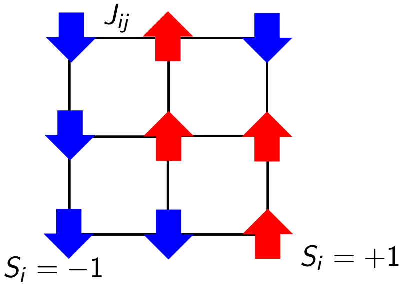
The Exact Algorithm for Hard Instances

Spinglass	Graph G=(V, E)
	 node of G
	 edge of G
coupling J_{ij}	edge weight c_{ij}
configuration	node partition V^+, V^-

The Exact Algorithm for Hard Instances



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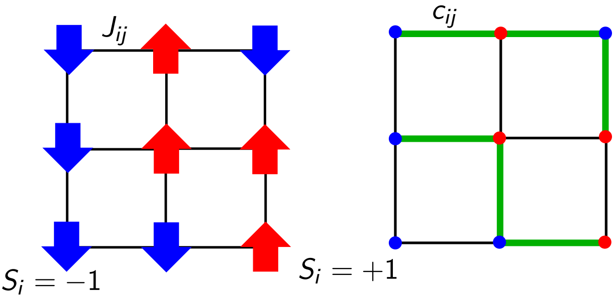
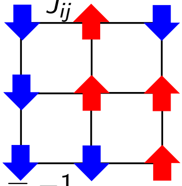
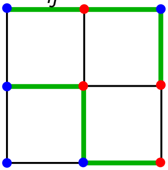


$G = (V, E)$

$H = -\sum_{e \in E} J_{ij} S_i S_j$

Computing Exact Ground States

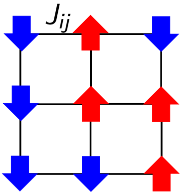


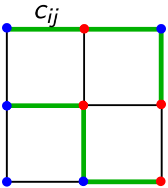


$$H(\underline{S}) + \sum_{(i,j)\in E} J_{ij} = \sum_{(i,j)\in E} J_{ij} \underbrace{(1 - S_i S_j)}_{= \begin{cases} 2 & \text{, if } S_i \neq S_j \\ 0 & \text{, otherwise} \end{cases}}$$

$$= 2 \sum_{S_i \neq S_j} J_{ij}$$

Computing Exact Ground States





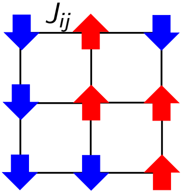
$$H(\underline{S}) + \text{const}$$

$$= 2 \sum_{S_i \neq S_j} J_{ij}$$

cut $= \{(i,j) \in E \mid (i,j) =$  $\}$

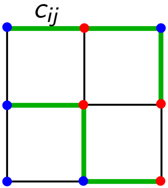
its weight: $\sum_{(i,j)\in\text{cut}} c_{ij}$

Computing Exact Ground States



$$H(\underline{S}) + \text{const} = 2 \sum_{S_i \neq S_j} J_{ij}$$

ground state min $H(\underline{S})$



cut $= \{(i,j) \in E \mid (i,j) =$  $\}$

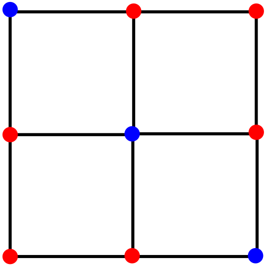
weight $\sum_{(i,j)\in \text{cut}} c_{ij}$

with $c_{ij} = -J_{ij}$:

maximum cut in G

NP-hard in general

Example



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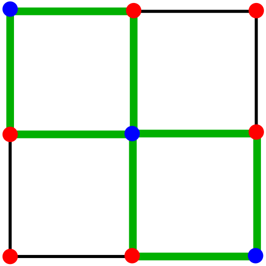

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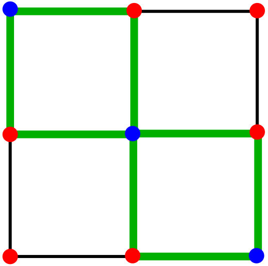

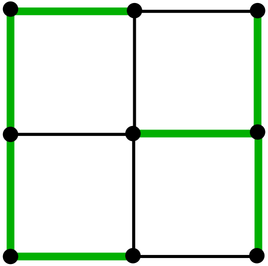

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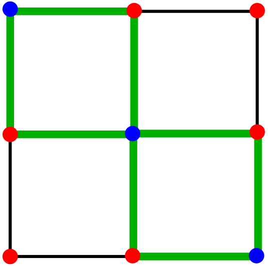

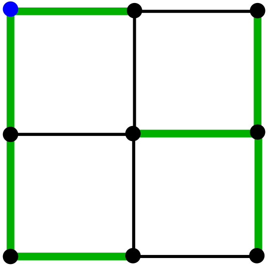

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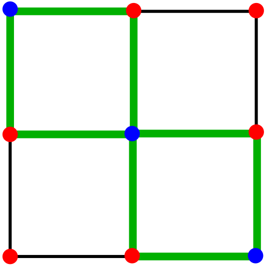

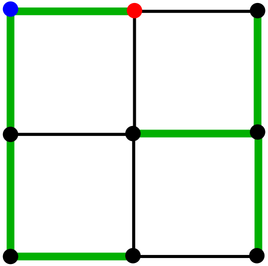

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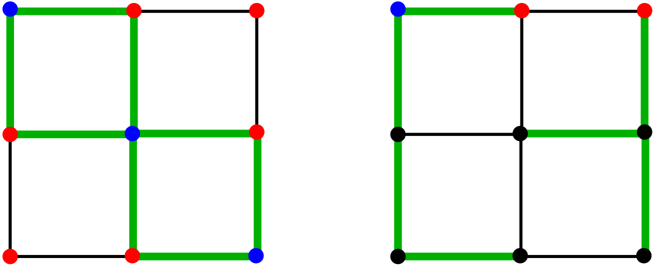

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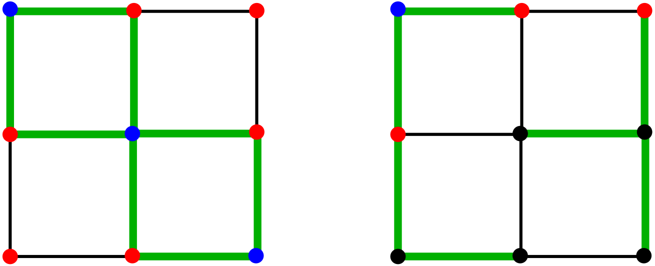

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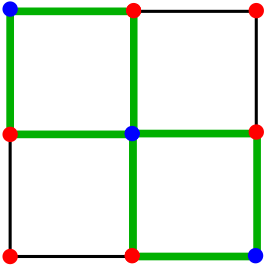

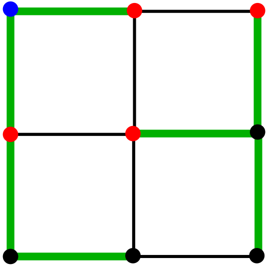

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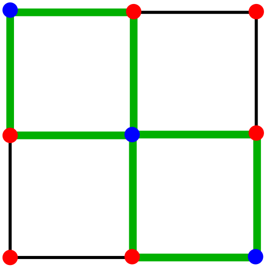

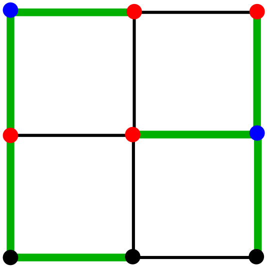

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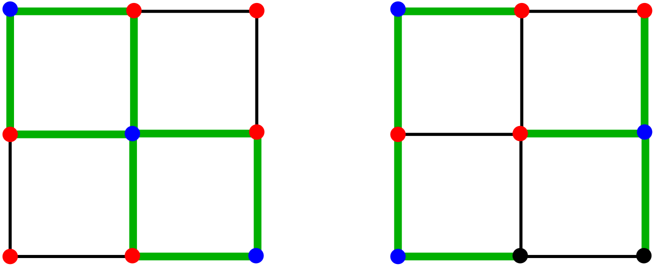

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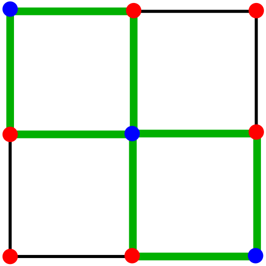

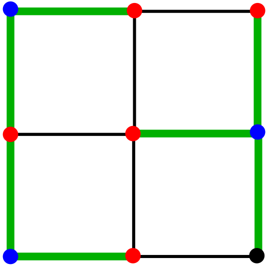

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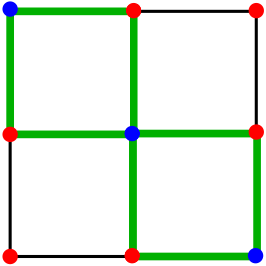

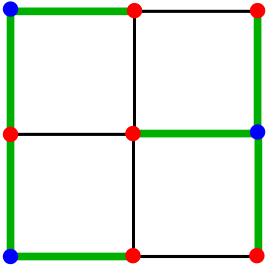

Branch-and-Cut

- is a clever enumeration method
- is a general framework for solving hard combinatorial optimization problems
- however: specification to a certain problem is science of its own
- for maxcut: started by M. Jünger, G. Reinelt, G. Rinaldi
- improved by M. Diehl, FL
- ground-state server via command-line client or web interface, get result by email (will be extended)

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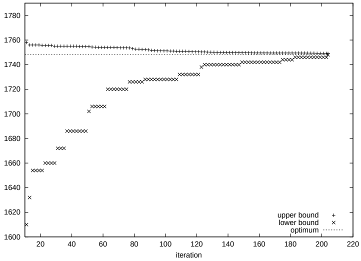
Branch-and-Cut Algorithm



- (lb): lower bound for optimum
- (ub): upper bound
- (lb) = (ub) $\Rightarrow$ optimality

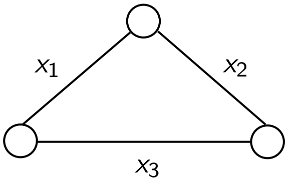
Calculation Of (ub) For Maxcut

$$(i,j) \in E \rightarrow 0 \leq x_{ij} \leq 1$$
$$(i,j) \in \text{cut} \rightarrow x_{ij} = 1$$
$$(i,j) \notin \text{cut} \rightarrow x_{ij} = 0$$

consider

$$P_C(G) : \text{convex hull of all cut vectors}$$

e.g. for



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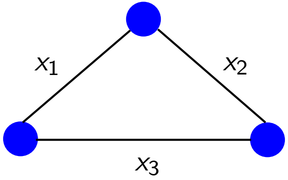

possible cut vectors:

$$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

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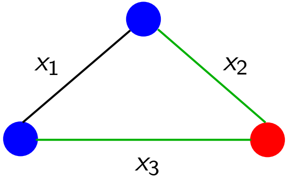

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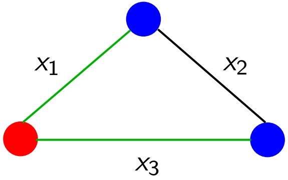

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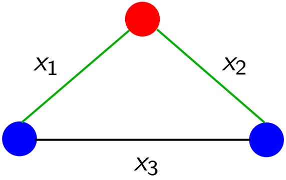
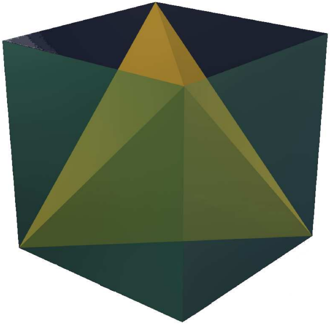


possible cut vectors:

$$\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

$$\mathrm{conv}\left\{\begin{pmatrix}0\\0\\0\end{pmatrix},\begin{pmatrix}0\\1\\1\end{pmatrix},\begin{pmatrix}1\\0\\1\end{pmatrix},\begin{pmatrix}1\\1\\0\end{pmatrix}\right\} =$$



cut polytope can be described by linear inequalities!

- however: in higher dimensions too many would be needed, not all known
- solution: find part of the necessary inequalities that can ‘easily’ be determined
- $\rightarrow$ optimize over a solution space P that contains cut polytope
- yields (ub)

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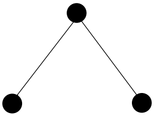
Branch And Cut Algorithm

FL, M. Jünger, G. Reinelt, G. Rinaldi, in 'New Optimization Algorithms in Physics', A.K. Hartmann and H. Rieger (Eds.), Wiley-VCH (2004).

1. start with some solution space $P \supseteq P_C(G)$
2. solve linear program

$$(\text{ub}) = cx^\star = \max \sum_{e \in E} c_e x_e, \qquad x \in P$$

3. (lb): value of any cut
4. if (ub)=(lb) or $x^\star$ is a cut: STOP
5. else: find better description P, goto 2)
6. if no better description can be found: BRANCH
   - select x_e with $x_e^\star \notin \{0;1\}$



$x_e = 0$ $\quad$ $x_e = 1$

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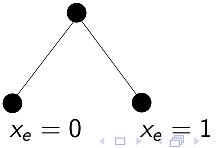

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2d Spin Glasses in a Field

with Olivier C. Martin (Paris)

FL, O.C. Martin, Physical Review B, **76**, 6 (2007).

spin glasses

- exhibit subtle phase transitions
- in 2d: $T_c = 0$, in 3d: $T_c > 0$
- their physics in 3d is not yet agreed upon
- their physics in 2d without a field agrees well with the scaling/droplet (DS) picture of Bray/Moore and Fisher/Huse (mid 80')
- for 2d with a field: previous studies found discrepancies to DS

Is DS correct for 2d spin glasses in a field?

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with Olivier C. Martin (Paris)

FL, O.C. Martin, Physical Review B, **76**, 6 (2007).

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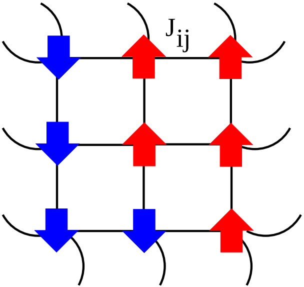
Our Approach

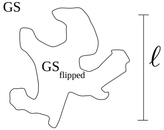
- exact ground-state algorithm
- study larger lattice sizes than before
- determine precise points where the ground states change as function of B
- study the properties of flipped clusters



- $L \times L$ lattice, periodic boundaries, Ising spins
- Gaussian/exponential J_{ij}
- $H(S) \equiv -\sum_{\langle ij \rangle} J_{ij} S_i S_j - B \sum_i S_i$

The droplet and scaling hypothesis

- low-lying excitations arise by droplet flips



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- $B = 0$: $y_T = -\theta$, y_T defined by $\xi \sim T^{\frac{-1}{y_T}}$
- $B = 0$: previous studies in 2d agree with DS and find $y_T = -\theta \approx 0.282$
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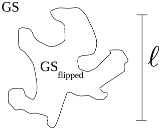

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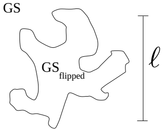

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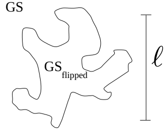

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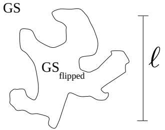

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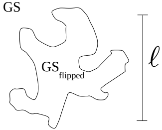

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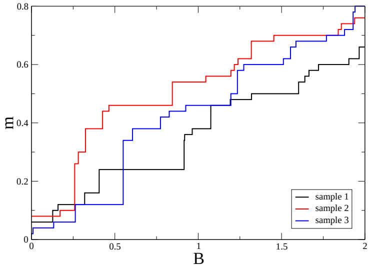
Details of our project

- Gaussian (and exponential) J_{ij}
- 2500 for $L = 80$, 5000 for $L = 70$, $2000 - 11000$ for $L \leq 60$



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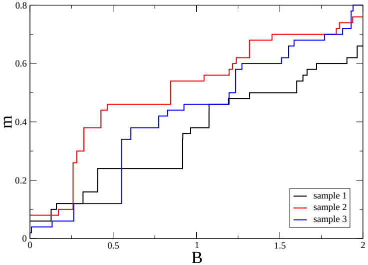

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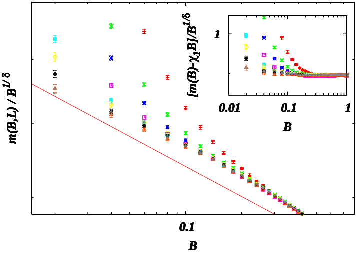

- however: no flat region for $L \rightarrow \infty$, as found earlier
- power-law fit yields $\delta = 1.45$ ($L = 50$)

- reason for discrepancy: m has analytic and non-analytic contributions: $m = \chi_1 B + \chi_S B^{1/\delta} + \ldots$, where $\chi_1 B$ cannot be neglected
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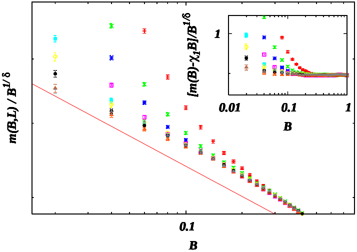

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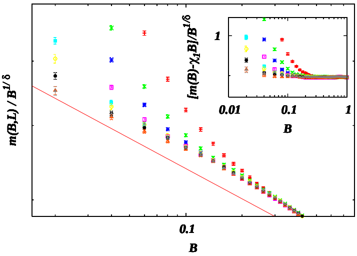

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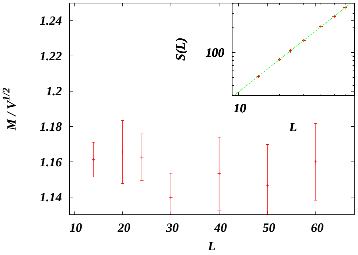
study for each realization of the disorder the largest cluster flipped for $B \in [0, \infty[$



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- their volume $V \sim L^2 \longrightarrow$ compactness
- $M/\sqrt{V}$ (M: cluster magnetization) insensitive to $L \longrightarrow$ random magnetization
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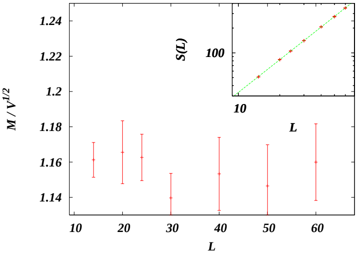

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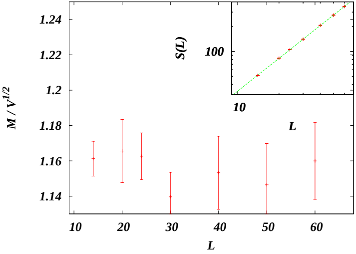

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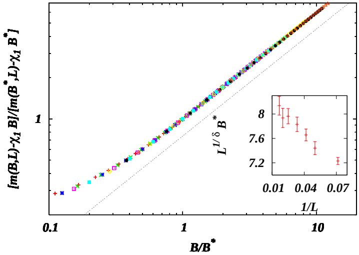

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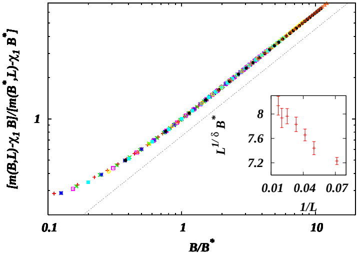

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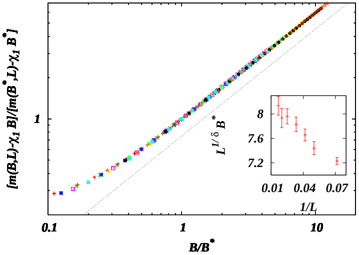

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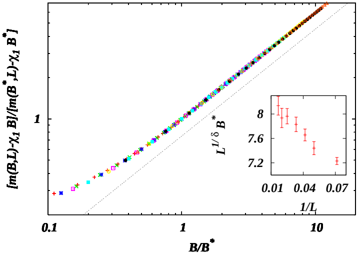

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We validated the predictions of the droplet/scaling picture:

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Outline

1. Hard Ising Spin Glass Instances
2. $2d$ Ising Spin Glasses in a Field
3. Potts Glasses
4. Potts Glasses with $q \to \infty$

Potts Glasses

with Bissan Ghaddar, Miguel Anjos (U. Waterloo, Canada)

B. Ghaddar, M. Anjos, FL (submitted)

- A spin can be in k different states $q_1, \ldots q_k$

Hamiltonian:

$$H = -\sum_{\langle i,j \rangle} J_{ij} \delta_{q_i q_j}$$

- we solve the problem also via branch-and-cut
- however: the bounds through linear optimization are very weak in practice and
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with Bissan Ghaddar, Miguel Anjos (U. Waterloo, Canada)

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Hamiltonian:

$$H = -\sum_{\langle i,j \rangle} J_{ij} \delta_{q_i q_j}$$

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semidefinite programming (SDP) problem: minimize a linear function of a symmetric matrix X subject to linear constraints on X, with X being positive semidefinite.

Branch-and-Cut Algorithm for Potts Glasses

at each node of the branch-and-cut tree:

1. use pos. semidef. optimization to obtain a LB
2. add valid inequalities to get a tighter LB
3. find a feasible solution to get an UB
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Results

$\|V\|$	Best Solution Value	Root Node LB	Root Node UB	Root Node Time	# of Nodes - Time to achieve 0%
5 × 5	-1484348	-1484722	-1484348	0:00:18	2 - 0:00:23
6 × 6	-2865560	-2865560	-2865560	0:05:12	1 - 0:05:12
7 × 7	-3282435	-3282435	-3282435	0:52:08	1 - 0:52:08
8 × 8	-5935341	-5935341	-5935341	2:21:43	1 - 2:21:43
9 × 9	-4758332	-4806178	-4758332	3:35:49	4 - 13:41:17
10 × 10	-6570984	-6630202.5	-6570984	10:36:23	6 - 18:09:41
11 × 11	-8586382	-9015701.1	-8586382	5:48:50	-
12 × 12	-10646782	-11189768	-10646782	9:31:00	-
13 × 13	-11618406	-12292274	-11618406	29:33:27	-
14 × 14	-13780370	-14607192	-13780370	47:16:57	-
2 × 3 × 4	-2197030	-2197030	-2197030	0:01:14	1 - 0:01:14
2 × 3 × 5	-2026448	-2026448	-2026448	0:08:02	1 - 0:08:02
2 × 4 × 5	-3392938	-3392938	-3392938	0:36:18	1 - 0:36:18
3 × 3 × 3	-1882389	-1882389	-1882389	0:00:21	1 - 0:00:21
3 × 3 × 4	-3192317	-3192317	-3192317	0:26:52	1 - 0:26:52
3 × 3 × 5	-4204246	-4209348	-4204246	2:52:31	5 - 3:38:37
3 × 4 × 4	-5387838	-5421403	-5387838	0:58:15	3 - 1:38:51
4 × 4 × 4	-7474525	-7529318	-7474525	3:22:37	3 - 10:12:11

Table: results for spinglass2g and spinglass3g instances where $k = 3$. The time is given in hr:min:sec.

Results

	$\|V\|$	$k=5$ Objective Value	$k=5$ Time	$k=7$ Objective Value	$k=7$ Time
spinglass2g	6×6	-2865560	0:23:41	-2865560	0:21:00
	7×7	-3843979	0:42:31	-3864156	0:39:23
	8×8	-5935341	2:09:07	-5935341	2:13:05
	9×9	-5745419	2:39:38	-6026024	2:18:56
	10×10	-6860706	19:14:02	-7644016	17:32:29
spinglass3g	$2 \times 3 \times 4$	-2212707	0:00:10	-2212707	0:00:08
	$2 \times 3 \times 5$	-2081357	0:08:07	-2081358	0:05:35
	$2 \times 4 \times 5$	-3578762	0:17:00	-3578762	0:13:01
	$3 \times 3 \times 3$	-2932403	0:00:47	-2932403	0:00:03
	$3 \times 3 \times 4$	-3552295	0:26:58	-3559337	0:21:15
	$3 \times 3 \times 5$	-4561622	2:04:49	-4648539	1:02:09
	$3 \times 4 \times 4$	-5371414	1:14:11	-5466518	1:18:02
	$3 \times 4 \times 5$	-5474952	24:49:15	-5530625	4:09:23
	$4 \times 4 \times 4$	-7619675	9:30:19	-7646881	4:57:05

Table: results for $k = 5$ and 7. The time is given in hr:min:sec.

doable sizes: ≤ 100 spin sites.

Although the doable sizes are small, we are not aware of a faster exact algorithm.

next step: replace the slow SDP-Solver by some faster routine

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Outline

1. Hard Ising Spin Glass Instances
2. $2d$ Ising Spin Glasses in a Field
3. Potts Glasses
4. Potts Glasses with $q \to \infty$

Potts Glasses with $q \to \infty$

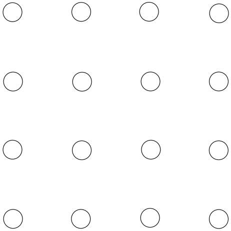
with Diana Fanghänel (Cologne)

D. Fanghänel, FL (in preparation)

Juhasz, Rieger, Iglòi (2001) have shown: for many states the dominant contribution to the partition function is

$$\max_{A \in E(G)} q^{f(A)},$$

$$f(A) = \text{number of connected components in } A(G) + \sum_{i,j \in A(G)} J_{ij}$$



$$f(A) = 16$$

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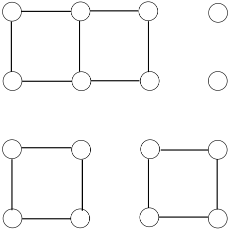

ass. $J_{ij} = 0.1 : f(A) = 5 + 15 * 0.1$

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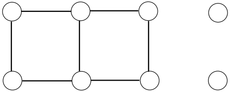
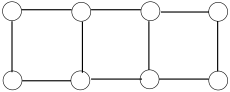


ass. $J_{ij} = 0.1 : f(A) = 4 + 17 * 0.1$



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- it uses many maximum-flow calculations (polynomial, but takes long)
- our work: reduce the number of maximum-flow calculations by graph-theoretic considerations

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use coupling strengths w_1, w_2 at criticality: $w_1 + w_2 = 1$

- number of maximum-flow calculations reduces by $\sim \frac{1}{3}$
- $L = 128$: ca 1.5 minutes cpu time
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from ‘difficult’ to ‘easy’:

system	currently treatable sizes
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3d Ising (w/o field)	$\sim 12^3$
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