Analytical and Numerical

Studies of Spin Glasses

Enzo Marinari

(Roma *La Sapienza*, Italy)

Disordered systems, spin glasses and structural glasses.

Analytic and numerical approaches to systems where *many states* play a crucial role (statics and dynamics).

Mainly as an example, recent results by T. Aspelmeier, A. Billoire, M. Moore and E.M., *Finite size corrections in the Sherrington-Kirkpatrick model* arXiv:0711.3445.

Eindhoven, March 2008

Main issues and ideas.

- Disordered and complex systems
- Spin glasses
- Analytic techniques and replica theory
- A very unusual landscape
- Numerical techniques: the example of Parallel Tempering.
- Finite size effects in the mean field theory of spin glasses

The physics of disordered and complex systems.

1. A small amount of (relevant) disorder can completely change the behavior of a (physical) system.

2. A "complex" deterministic Hamiltonian can produce exactly the same behavior of a disordered system. (Derrida REM vs. Bernasconi autocorrelation).

   Mézard-Parisi approach.

3. Large and very different classes of problems are of this kind.

   Optimization, for example. Use the same approach for understanding, improving, solving...

Deriving the properties of such a system is difficult (still, crucial analytic frame derived by Parisi with RSB).

Both analytic studies and numerical studies are not an easy task (for similar reasons).

"Best solution" ($T = 0$, ground states, energy) can be complex,
"good solutions" ($T > 0$ landscape, typical configurations, free energy) can be complex.

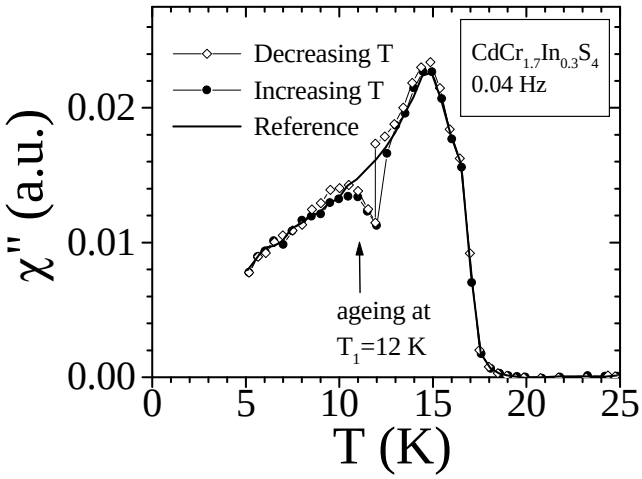
Materials, optimization problems, social systems.

Spin glasses have been, in the last years, lucky materials.

They are not very interesting from any technological point of view. Still, some people care a lot about them.

But: very interesting and new phenomena. And a very interesting theory. From material physics to structural glasses, and a paradigmatic role leading to optimization, games, disorder in biological systems.

Look at this experiment.



These features are natural in a hierarchical valley approach (but very possibly are not explained by models, see later...).

The paradigm

- Financial markets

  Players with pools of (random) strategies

  They minimize a cost function (Hamiltonian)

- Satisfiability

  K-SAT

  N Boolean variables $\{x_i\}_{i=1,N}$, $x_i \in \{0,1\}$

  M clauses (constraints) $C_1, \ldots C_M$ consisting of the OR of 3 distinct variables (or of their negations)

  Example: $x_3 \vee \overline{x_{12}} \vee \overline{x_{24}}$

  For a given assignment of the x_i, a clause is TRUE or FALSE

  $\exists$ assignment $\{x_i\}_{i=1,N}$ such that $F(\{x_i\})$ is TRUE?

- Biophysics

  Heterogeneity

  Stoichiometry

The standard model (maybe not really correct...):

$$H_{EA} \equiv - \sum_{\text{i nn j}} \sigma_i J_{ij} \sigma_j \ ,$$

Edwards-Anderson spin glass. $\sigma_i = \pm 1$ (or Heisenberg), sum is over first nearest neighboring sites, in D spatial dimensions.

$P(J) \sim e^{-J^2}$ or $J = \pm 1$ with probability $\frac{1}{2}$.
Random couplings are quenched: that gives the huge complexity.

One cannot solve this model (one cannot even more or less understand it...). So define mean field theory:

$$H_{SK} \equiv - \sum_{\text{all couples i j}} \sigma_i J_{ij} \sigma_j \ ,$$

where the sum runs now over all spin couples (Sherrington and Kirkpatrick).

The mean field theory can be solved, and it shows a really peculiar behavior. Recently a mathematical proof of the correctness of the solution has been obtained (Talagrand building on Guerra work).

Which kind of random disorder?

Couplings $\{J\}$.

"Fixed disorder" (that does not change on the time scales we are considering). Compute Z_J and average the free energy:

$$\overline{\log Z_J}$$

Very different from

$$\overline{Z_J}$$

(annealed case), and far more interesting.

But more difficult.

How can we compute $\overline{\log Z_J}$?

Parisi mean field solution. Use replicas.

$$\log Z = \lim_{n \longrightarrow 0} \frac{Z^n - 1}{n} \ ,$$

and defining with the over-line $\bar{\cdot}$ the (quenched) disorder average:

$$\overline{\log Z} = \lim_{n \longrightarrow 0} \frac{\overline{Z^n - 1}}{n} \ ,$$

So compute $Z(n)$ from Z, Z^2, Z^3, ..., $Z^{(1)} \cdot Z^{(2)} \cdot Z^{(2)} \cdot$ ..., and define $\lim_{n \longrightarrow 0}$ from analytic continuation of $Z(n)$.

Natural guess: in $Z^{(1)} \cdot Z^{(2)} \cdot Z^{(3)} \cdot$ ... all replicas are symmetric.

Parisi: replica Symmetry undergoes spontaneous symmetry breaking.

A complex phase space emerges.

Replicas

Disorder makes things far more difficult, already at mean field level.

After some work one finds that $\overline{Z^n}$ (and lim for $n \to 0$) can be obtained as a solution of a saddle point problem with a function (for $h = 0$, $E(J) = 0$)

$$\sum_{(\alpha\beta)} \frac{1}{2} y_{(\alpha\beta)}^2 - \log \ \mathrm{Tr}\ e^{\beta J \sum_{(\alpha\beta)} y_{(\alpha\beta)} \sigma_\alpha \sigma_\beta}$$

with

$$\alpha = 1, \cdots, n \ , \quad \beta = 1, \cdots, n \ , \quad \alpha \neq \beta \ , \quad n \to 0$$

and $y_{(\alpha\beta)}$ is a 0×0 matrix.

Replica Symmetry.
Assume $y_{(\alpha\beta)} = y$ for each $(\alpha\beta)$ (looks natural, since replicas are a mathematical artifact to start with).

Solution is correct for $T > T_c$, but wrong for $T < T_c$.

Replica Symmetry is broken!

Parisi solution is needed. Parisi solution by iteration.
Replica symmetry: $n \times n$ matrix.

$$y = \begin{pmatrix} 0 & y_0 & y_0 & y_0 & y_0 & y_0 \\ y_0 & 0 & y_0 & y_0 & y_0 & y_0 \\ y_0 & y_0 & 0 & y_0 & y_0 & y_0 \\ y_0 & y_0 & y_0 & 0 & y_0 & y_0 \\ y_0 & y_0 & y_0 & y_0 & 0 & y_0 \\ y_0 & y_0 & y_0 & y_0 & y_0 & 0 \end{pmatrix}$$

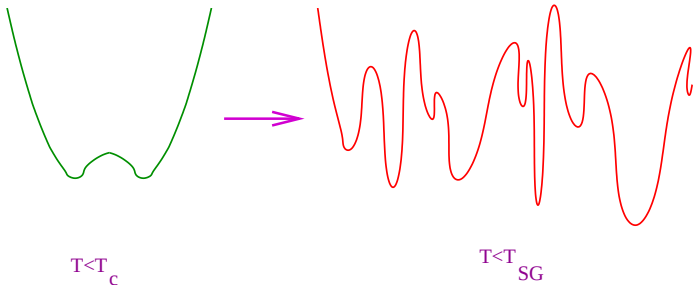
Variational problem in one parameter y_0.
We need something less trivial.
First step. Break the $n \times n$ matrix into $n/m_1 \times n/m_1$ blocks of size $m_1 \times m_1$. Change y_0 in y_1 on diagonal blocks and leave the off-diagonal blocks unchanged.

$$y = \begin{pmatrix} 0 & y_1 & y_1 & y_0 & y_0 & y_0 \\ y_1 & 0 & y_1 & y_0 & y_0 & y_0 \\ y_1 & y_1 & 0 & y_0 & y_0 & y_0 \\ y_0 & y_0 & y_0 & 0 & y_1 & y_1 \\ y_0 & y_0 & y_0 & y_1 & 0 & y_1 \\ y_0 & y_0 & y_0 & y_1 & y_1 & 0 \end{pmatrix}$$

Now: three parameters (y_0,y_1 andm_1). One step.
Stable for "glassy models".
Do it again, two steps. Three, four,....
∞ number of steps is stable and correct solution for spin glasses.

Main features of Sherrington-Kirkpatrick, Mean Field Spin Glasses phase space.

1. Complex phase space:

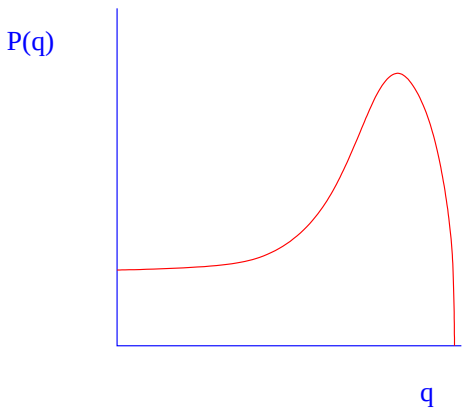


2. This situation implies the phase transition also exists for $h > 0$.

3. Two microscopic configurations of the system at equilibrium can be very similar or very different. Measure the overlap

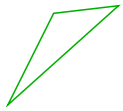
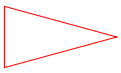
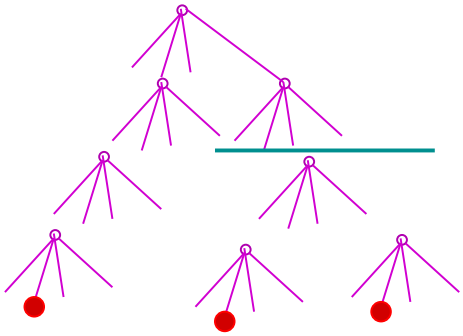
$$q \equiv \frac{1}{N} \sum_i \sigma_i^{(\alpha)} \sigma_i^{(\beta)} \ .$$

$P(q)$ has measurable support when $N \longrightarrow \infty$ for $T < T_c$.



4. States that characterize the system at equilibrium obey an ultrametric inequality for the distance:

$$\delta^{\alpha\beta} \simeq 1 - q^{\alpha\beta} \equiv 1 - \frac{1}{N}\sum_i \sigma_i^{(\alpha)}\sigma_i^{(\beta)}.$$

So, not only triangular inequality:  (obvious since δ is a distance) but also UM inequality. All triangles are isosceles with two equal sides longer than the shortest side. They can be equilateral (same state).  States turn out to be organized on a ultrametric tree.  How much of this is shared from 3D spin glass? This is not clear (I would say much) but maybe it is not too relevant (very relevant systems in many contexts are mean field like in nature).

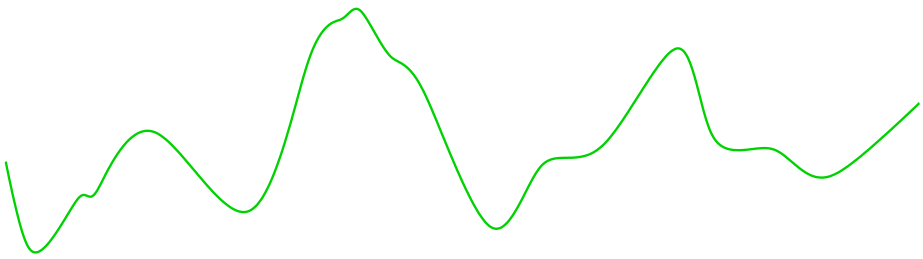
A theoretical "very complex" structure is nowadays well understood.

Optimized Monte Carlo Methods: Parallel Tempering

For Tempering and Parallel Tempering see: EM and Parisi 1992, Tesi et al. 1995; Geuer and Thompson 1994; Hukushima et al. 1995.

Free Energy Barriers

This is a Complex Free Energy landscape



Normal Monte Carlo cannot and does not work.
Difficult to cross. Crucial to cross.
If we change T free energy barriers change. When T increases barriers become smoother and smoother. When T reaches T_c the landscape has been flattened.

Idea: let the system walk in temperature space, going down to the low, interesting T value, and up all the way, through a chain of intermediate T values up to some $T \gg T_c$.

(A bit like annealing, but needs to be always at thermal equilibrium: tempering is annealing for free energy).

Generic class of methods where you modify the probability distribution π:

$$\int \pi O \sim \int \nu O' \ , \quad \text{where } \nu = \frac{\pi}{\rho} \ , \quad O' = \rho O$$

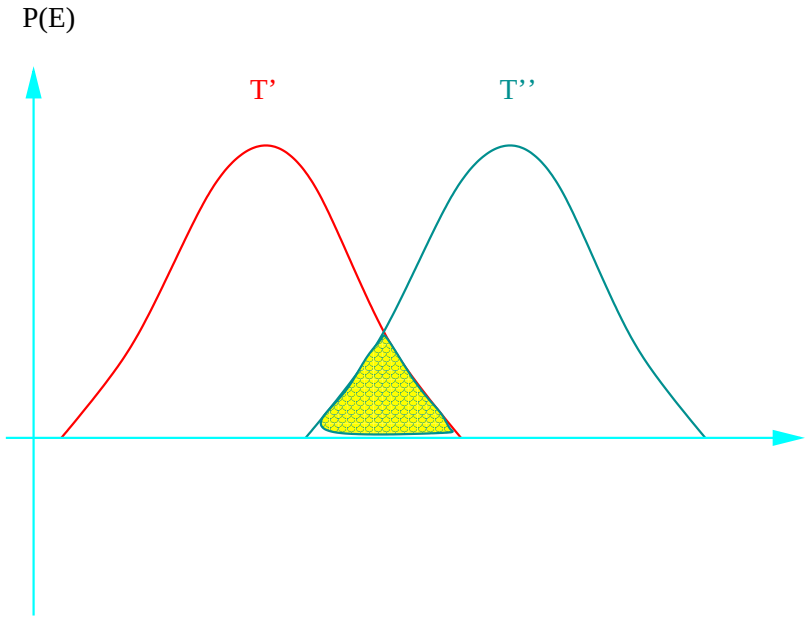
density scaling or umbrella sampling

Here the method is very simple since you have exactly the Boltzmann distribution at each T value (no reconstruction is needed: just select data at the correct T value). The method:

- select a discrete set of T values, $T_{(\alpha)}$: $\alpha = 0, 1, 2, \ldots, M$. Here $T_0 = T_{\text{min}}$ (typically smaller than T_c) and $T_M = T_{\text{max}}$ (typically larger than T_c).
- Clone your system M times, i.e. consider M configurations C_α of your system.
- start by assigning $T(C_0) = T_0$, $T(C_1) = T_1$, $\ldots$, $T(C_M) = T_M$.
- go ahead with Monte Carlo sweeps.

Two parts of Monte Carlo sweep:

- Usual MC sweeps on all copies of the system at fixed temperature.
- Swap two values of T. Consider $C(T_0)$ and $C(T_1)$. Propose them to swap T values.



Selection of T values range and spreading is the freedom of the method. If equidistributed T values and T_{min} is fixed from physics parameters are N_T and ΔT.

Use Metropolis to swap

$$\Delta S \equiv S' - S = \left(\beta' E + \beta E\right) - \left(\beta E + \beta' E'\right)$$

- do previous point for all configuration couples $C(T_1)$ and $C(T_2)$, $C(T_2)$ and $C(T_3)$ etc.

Choice of

- $T_{\min}$: interesting physics + reasonable CPU time.
- $T_{\max}$: "$\gg$" T_c.
- N_T: keep high acceptance factor for tempering swap.

Check thermalization

- Symmetry of $P_J(q)$ (here this is not as a strong check as in normal Monte Carlo: spin flip is not the slowest mode anymore).
- Check convergence of observables on logarithmic time scale.
- Check that acceptance rate for tempering has been kept high (see earlier).
- Each of the N_T copies of the system must have covered the $T_{(\alpha)}$ space with "many visits".

Multicanonical methods (B. Berg et al.) can deal with a number of general situations, since you can change in a complex way the a priori probability distribution (control for example first order phase transitions).

For spin glasses multicanonical methods have probably a slightly lesser performance than parallel tempering.

Replica MC algorithm by Swendsen and Wang: very effective in 2D (better than PT), comparable to PT in 3D.

Open problem: find an effective "clustering method", like Swendsen-Wang for Ising model.

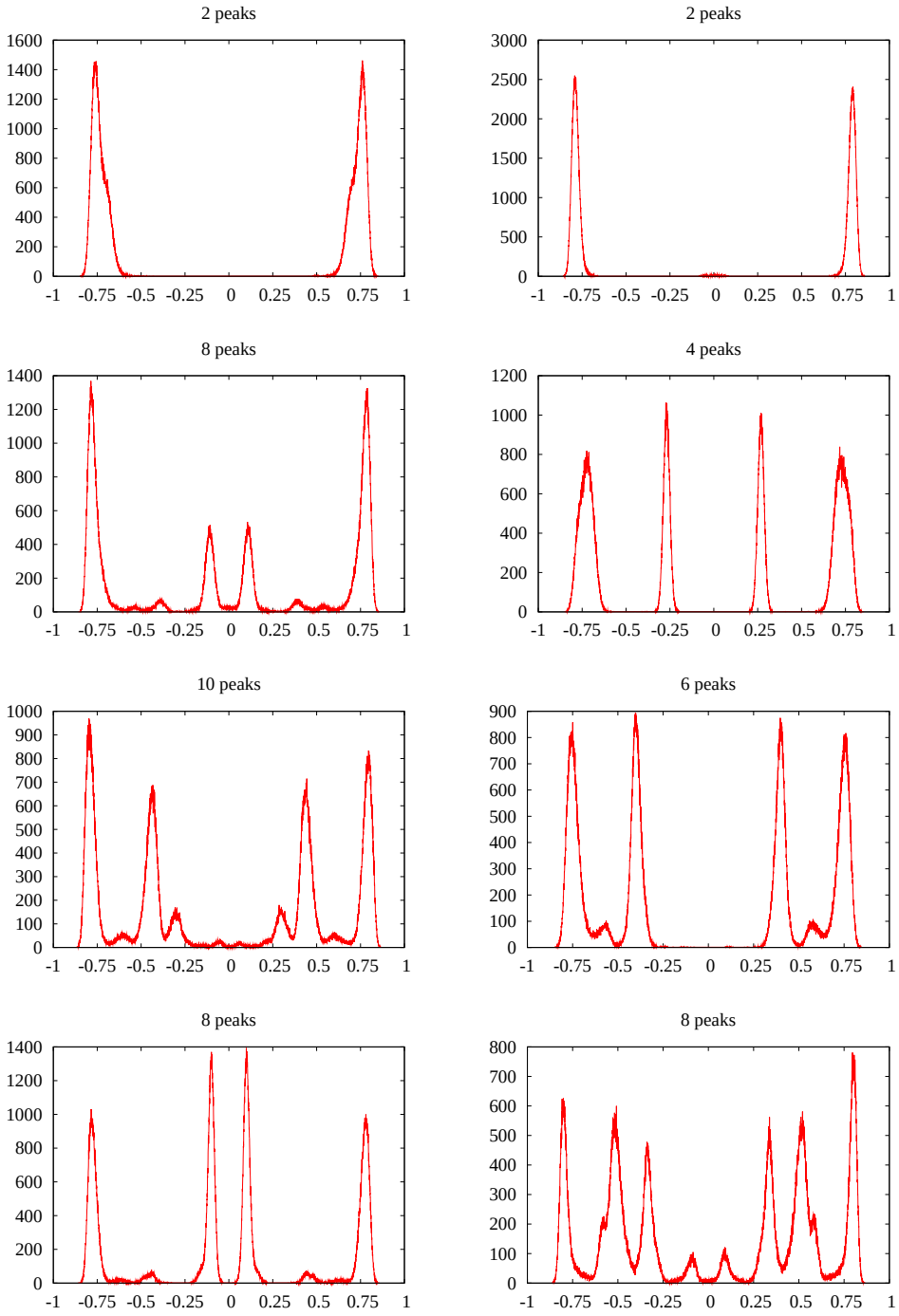
Finite size corrections in the Sherrington-Kirkpatrick model, T. Aspelmeier, A. Billoire, M. Moore and E.M., `arXiv:0711.3445`.

An example of results that can be obtained by joined analytic and numerical advances.

1. Finite size effects.
2. Sample to sample fluctuations.
3. Number of peaks and number of states.

$$P_J(q)$$

for a given disorder sample.



$P_J(q)$ for eight different disorder realizations: here $N = 4096$ and $T = 0.4000$. The symmetry of the plots around $q = 0$ is a good test of thermalization.

Even at finite N the function $P_J(q)$ (many peaks) is very different from the disorder average $\overline{P_J(q)}$ (one plateau and one peak close to the maximum of the support).

We study numerically the average number of peaks of $P_J(q)$ as a function of the system size N:

$$R_N \sim N^{\mu}$$

and find that the numerical results are compatible with the value $\mu \sim \frac{1}{6}$ that we expect from an analytic argument.

From this result we are able to derive a number of physical properties of the system.

We argue that:

finite N is equivalent to K steps (finite) in Parisi scheme.

We use this fact to connect μ to finite size effects, and to deduce their scaling behavior.

Use (accurate) numerical simulations to check these ideas, and to find that they do indeed work.

For example for the internal energy density:

$$e = e_{K=\infty,N=\infty} + de_N = e_{K=\infty,N=\infty} + O(K^{-4})$$

and since we find that $K \sim N^{\frac{1}{6}}$ we expect that $de_N \sim N^{-\eta} \sim N^{-\frac{2}{3}}$.

Numerical simulations and Monte Carlo methods are crucial when working on arguments that are very suggestive but not a theorem.

Numerical data support that $\eta = \frac{2}{3}$.

A sketch of the analytic argument.

Correlation function:

$$G_R(x,y) = \overline{\langle \sigma_x \sigma_y \rangle_c^2}$$

single valley replicon correlation function.

Fourier space. At Gaussian order:

$$G_R(k) \sim k^{-2}$$

for $T < T_c$ and $T = T_c$.

Divergence at $k = 0$, $\xi \longrightarrow \infty$
($m \sim \xi^{-1}$, and for $T > T_c$ we have that
$G(k) \sim (k^2 + m^2)^{-1}$).

At finite N no zero mass (no phase transition in finite volume, no infinite correlation length), and

$$m_{(N)}^2 \sim N^{-\frac{1}{3}}$$

At finite K and infinite volume you also have a finite mass

$$m_{(K)}^2 \sim K^{-2}$$

This implies

$$K \sim N^{\frac{1}{6}}$$

When K, level of Parisi breaking, is large enough in finite volume stability does not demand to increase it further.

Now: since $K \sim N^{\frac{1}{6}}$ we can use finite K expansions to compute finite size corrections.

For example:

$$\Delta u = \left(\frac{1}{2}t^2 + \frac{5}{6}t^3 + \frac{1}{3}t^4\right) - \frac{1}{72}t^4\left(\frac{1}{K}\right)^4 + \cdots$$

and the Edwards-Anderson order parameter is to order K

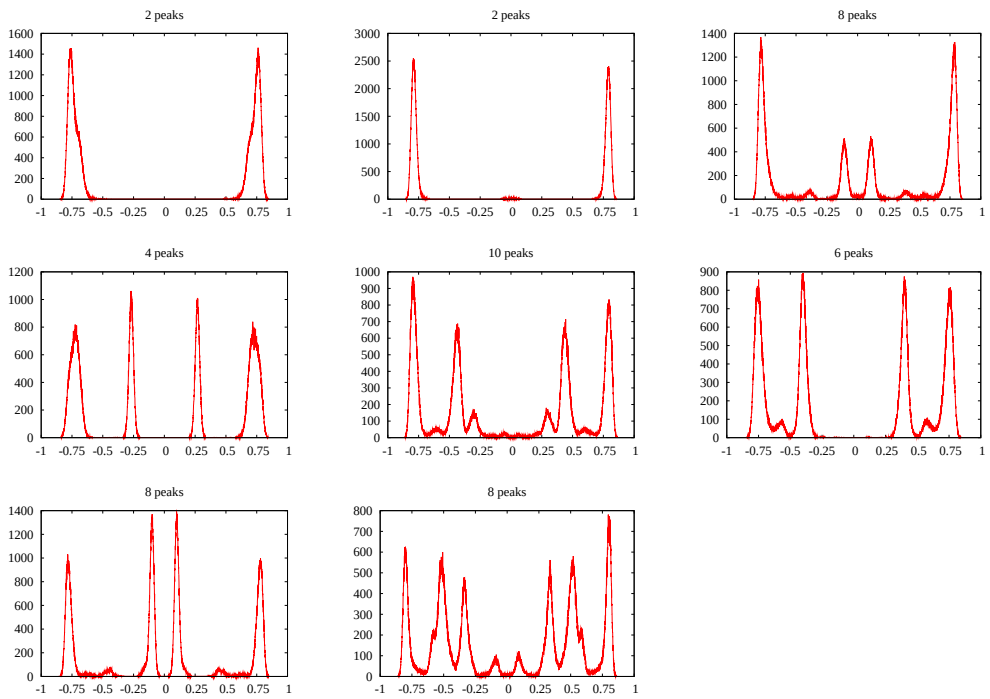
$$q_{EA} = t + t^2 - \frac{2}{3(2K+1)^2}t^2 \ .$$

Numerically:

- Parallel tempering.
- N up to 4096.
- T down to less than $\frac{T_c}{2}$.
- N_T up to 100.
- Thermalize and check thermalization. Detailed checks.
- $J = \pm 1$, binary couplings.
- Multi-spin coding.

Counting peaks is technically not easy.

The same figures we have seen before:



What is a "peak" if data are noisy?

Local maximum (after smoothing), with care of additional details.

Top figure on the left: two or four peaks?

Details become maybe irrelevant when N and R are very large, but we can only go up to $N = O(10^4)$ where R is small.

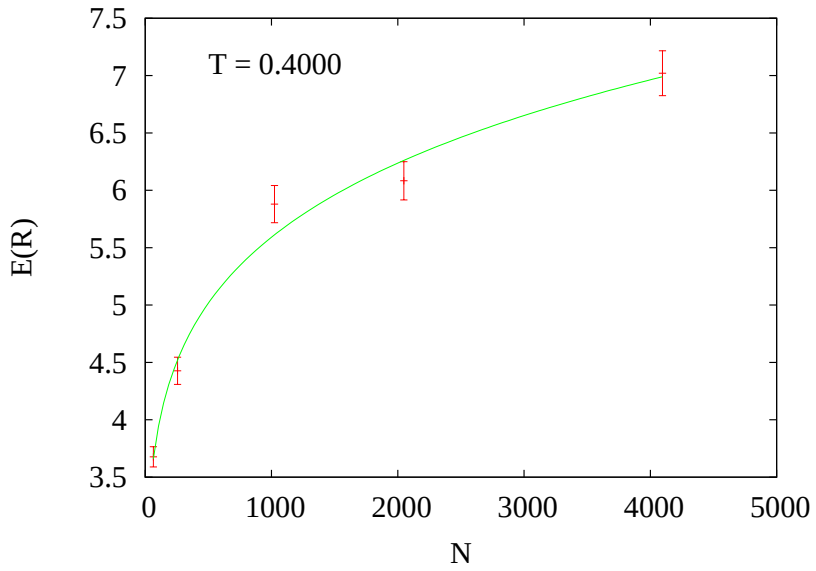


Figure 1: Scaling plot of $E(R)$ (the average number of peaks/features determined by visual inspection of the individual $P_J(q)$) as a function of N, for $T = 0.4$. The curve is the best fit to the form $E(R) = a + bN^c$ with $c = 0.17 \pm 0.14$.

Very large error, but the exponent is compatible with the value 1/6.

Finite size shift in physical observables

The energy

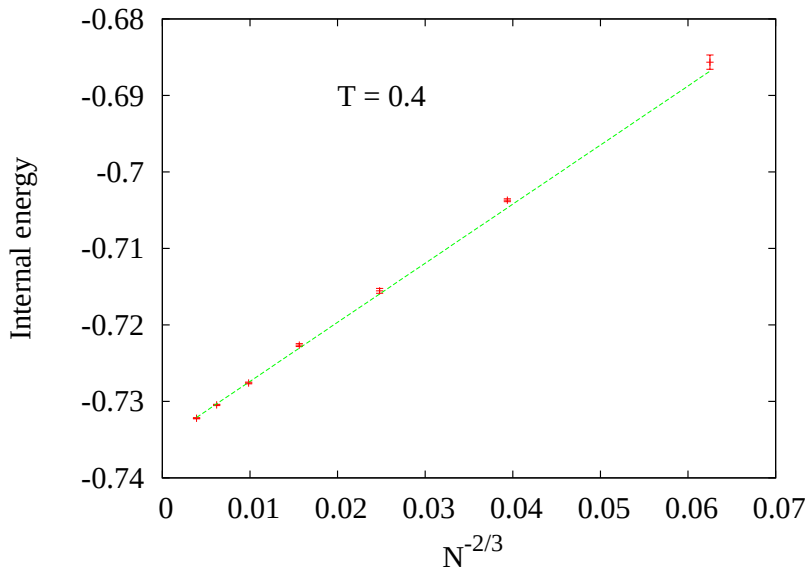


Figure 2: The internal energy as a function of $N^{-2/3}$ for $T = 0.4$. The line is a linear fit (using data for $N \geq 256$) as a function of $N^{-2/3}$ to the data.

q_{EA}

(see also work by Billoire, Franz and EM, J. Phys. A **36**, 15 (2003)).

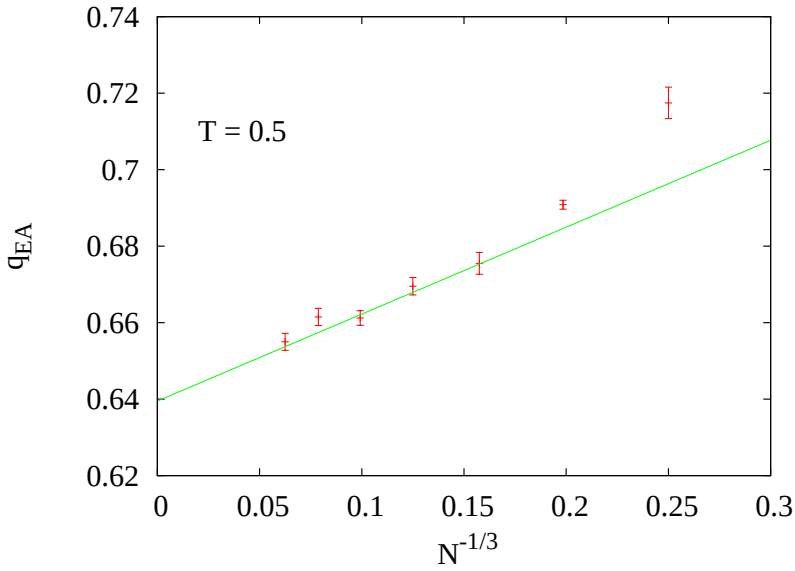


Figure 3: The Edwards–Anderson order parameter $q_{EA}(N)$, as defined in the text; here $T = 0.5$. The line is for the best fit to the data as a linear function of $N^{-1/3}$ (for $N \geq 256$).

Complex procedure for reconstructing q_{EA}.

Here as our analytic argument suggests finite size effects are of order $N^{-\frac{1}{3}}$.

Sample to sample fluctuations of the free energy and of the internal energy.

We are interested in:

$$\delta F^2 = N^2 \Big(E(\langle f \rangle_J^2) - E(\langle f \rangle_J)^2 \Big) \sim N^{2\Upsilon} \ .$$

Our theoretical approach suggests that Υ should be equal to $\frac{1}{6}$. We are also interested in:

$$\delta U^2 = N^2 \Big(E(\langle e \rangle_J^2) - E(\langle e \rangle_J)^2 \Big) \ .$$

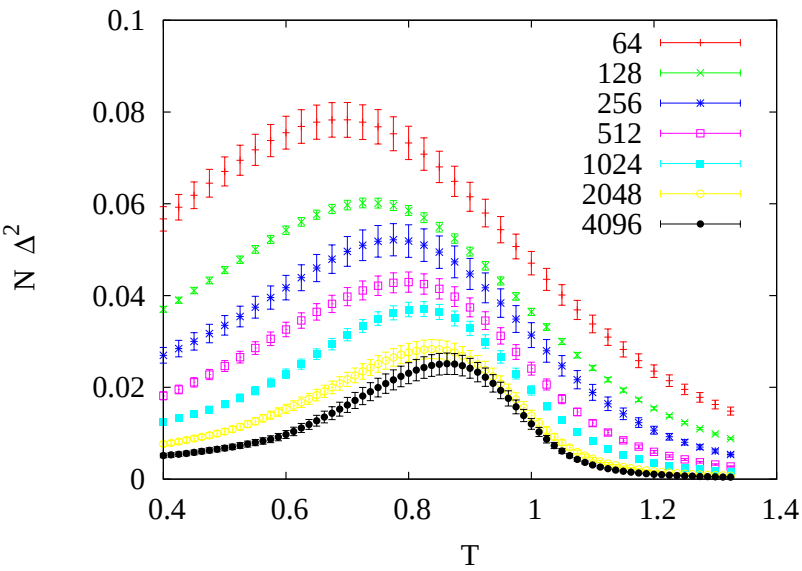


Figure 4: The energy fluctuation $\delta U^2/N = N\Delta^2(T)$ as a function of T, for different values of N.

Effective exponent. Difficult analysis, large finite size effects, but important evidence.

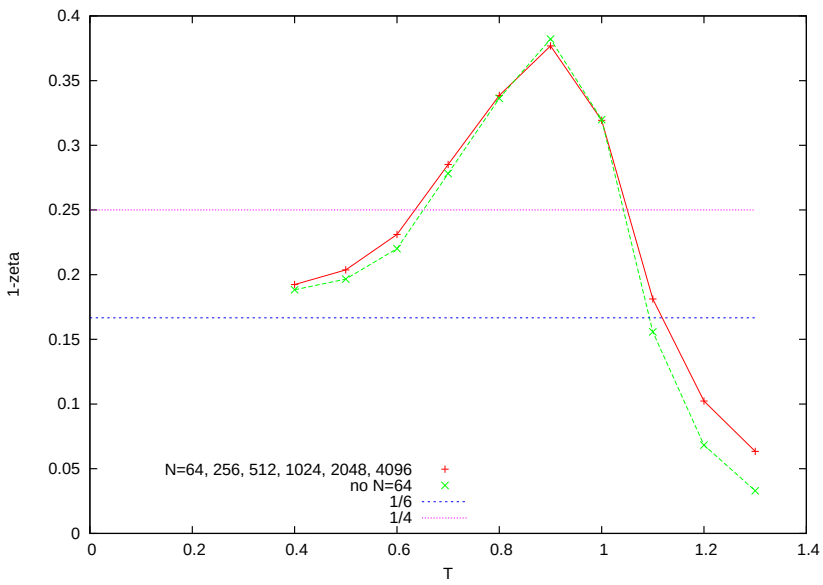


Figure 5: Exponent $1 - \zeta$ as a function of T. We show with the continuous lines the results of two best fits, one including all vales of N and the other including only values $N \geq 128$.

The end.

Computing Ground States.

Here ground states are (very) interesting.

- Optimization: solution.
- Statistical Mechanics: interesting physics, connected to low T physics.

Different approaches to ground state computation:

- Exact. Very effective in $2D$ with at least one open boundary. Very limited in $3D$.
- Heuristics: typically population dynamics, genetic algorithms, many scales and renormalization.

The exact algorithm.

Mainly useful in $2D$ (but now maybe also in $3D$).

Map the problem of finding the ground state of a spin glass in a max-cut problem (generically hard, i.e. difficult, i.e. complete, i.e. you do not have an algorithm for solving it in polynomial time in N).

Cut of a graph $G = (V, E)$ (vertexes, edges) is a partition of its vertexes into two disjoint subsets $V_1, V_2 \subset V$ and the implied set of edges between the two parts (each edge can carry a weight w_e, and the total weight of the cut is $w(C)$).

Max Cut (min Cut): divide vertexes in two parts so that total weight of edges between the two parts is max (min).

Generating function of cuts: polynomial

$$\sum_{\text{over all cuts}} x^{w(C)} .$$

From Ising to Cuts

Assign spins to $+1$ or -1.

$V_+ = \{i \in V | \sigma_i = +1\}$ $V_- = \{i \in V | \sigma_i = -1\}$.

Let $C(V_+, V_-)$ be the cut of spins $+1$ and -1.

$W \equiv \sum_{\{i,j\} \in E} J_{ij}$ is the sum of all edge weights in G.

$$H = \sum_{\{i,j\} \in C} J_{ij} - \sum_{\{i,j\} \in (E-C)} J_{ij} = 2w(C) - W$$

Let the generating function of cuts be

$$\mathcal{C}(G, x) = \sum_{\text{cuts in G}} c_k x^{w(C)} ,$$

where c_k is the number of cuts with weight k.

$$\begin{aligned} Z(\beta) &= \sum_{\{\sigma\}} e^{-\beta H} \\ &\simeq \sum_{\text{cuts}} e^{-2\beta w(C) + \beta W} \simeq e^{\beta W} \mathcal{C}(G, e^{-2\beta}) \end{aligned}$$

Finding the best cut you find the SG ground state.

Heuristic approach to GS computation

For example Pal, Houdayer-Martin, EM-Parisi, Palassini-Young, building on Kernighan-Lin, Kawashima-Suzuki.

- Local Search.
- Families $\Longrightarrow$ genetic selection.
- Renormalization.

Local Search Flip if "gain". Single spin flip, double spin flip...

Renormalization

$$H \equiv -\sum \sigma_i J_{ij} \sigma_j - \sum h_i \sigma_i \ .$$

Consider K such spin configurations (tentative ground states...): $\sigma_i^{(\alpha)}$. Compare these configurations, use block spins, and use their similarities/differences to update them.

Population Dynamics A genetic algorithm allows to select/improve/variate the K configurations.

Children tend to be better than parents (but keep variability!).

3-Sat

Here one (very important!) example among many: K-SAT (much more, all very connected: matching problems, traveling salesman, ...).

N Boolean variables $\{x_i\}_{i=1,N}$ $\quad x_i \in \{0,1\}$

M clauses (constraints) $C_1, \ldots C_M$ consisting of the OR of 3 distinct variables (or of their negations).

Example: $x_3 \vee \overline{x_{12}} \vee \overline{x_{24}}$

For a given assignment of the x_i, a clause is TRUE or FALSE

Decision problem (SAT)

$\exists$ assignment $\{x_i\}_{i=1,N}$ such that $F(\{x_i\})$ is TRUE?

Optimization problem (MAX-SAT)

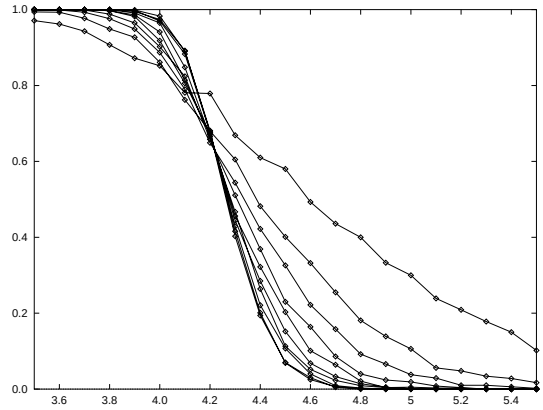
Find an assignment $\{x_i\}_{i=1,N}$ which minimizes E_{GS} = the number of FALSE clauses

The problem can be written in terms of a Statistical Mechanical Hamiltonian, making it very similar to a Spin Glass.

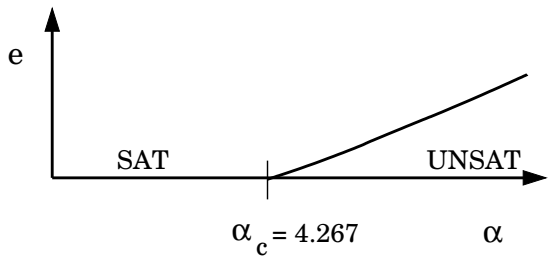
Random 3-Max-Sat

Each clause is chosen at random with the flat distribution among the $2^3 N(N-1)(N-2)/3!$ possibilities.

SAT-UNSAT phase transition

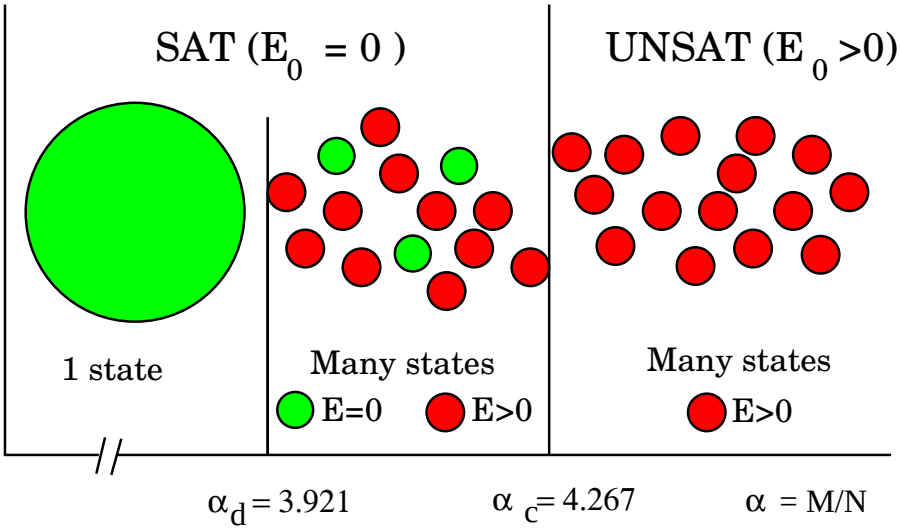


Probability that a random sample is satisfiable versus the control parameter $\alpha = M/N$



Ground state energy density $e = E_{GS}/N$ versus α

Statistical description of the clustering

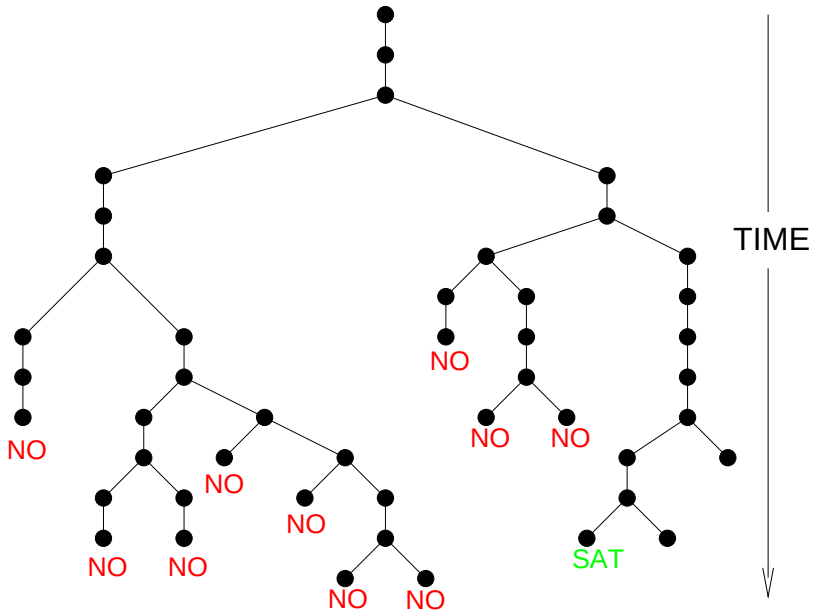


Mézard, Parisi, Zecchina and coworkers.

- Order parameters
- Organization of the ground states (para, spin glass,...)
- Energy landscape ($E > E_{GS}$, barriers, ...)
- Thermodynamics ($T > 0$)

Computational approaches

Checking for Sat or UNSAT:
Davis-Putnam-Loveland-Logemann algorithm



- Start with all x_i unassigned.
- BRANCHING: select one index i and branch ($x_i = 0$ and $x_i = 1$) and treat each sub-problem separately.
- PRUNING: if a node leads to one or more clauses being FALSE, label the node "NO" and backtrack. If no backtracking is possible, go to END.
- EXIT at a node if all clauses are TRUE (SAT sample).

END: If all leaves have been examined or pruned and are all labeled "NO", the sample is UNSAT.

Tool for solution of 3-SAT: belief propagation.

Can be improved dramatically, by understanding details of Replica Symmetry Breaking: survey propagation (by Mézard, Parisi and Zecchina, Science 2002).

Thousand-fold increase in the size of practical problems that can be solve (Mézard, Parisi and Zecchina, Mézard and Zecchina, PRE 2002, Brauenstein, Mézard and Zecchina, cs.cc/0212002).

Very interesting: use all what you know about the solution to derive an algorithm (see Swendsen and Wang with cluster algorithm based on properties of the Fortuin-Kasteleyn representation of the Ising model partition function).

Let $t_{i\to a}$ be the probability that variable x_i satisfies clause a in a solution.

Let $i_{a\to i}$ be the probability that clause a is satisfied by another variable than x_i.

Belief propagation gives in one direction the following iterative update equation:

$$i_{a\to i}^{(l)} = t_{j\to a}^{(l)} + t_{k\to a}^{(l)} - t_{j\to a}^{(l)} t_{k\to a}^{(l)} \ .$$

For the belief propagation equations in the other direction define

$$A_i^0 = \prod_{b\in V_i,\, y_{i,b}=\neg x_i} i_{b\to i} \ ,$$

$$A_i^1 = \prod_{b\in V_i,\, y_{i,b}=x_i} i_{b\to i} \ .$$

Update equations are

$$t_{i\to a}^{(l)} = \begin{cases} \dfrac{i_{a\to i}^{(l-1)} A_i^1}{i_{a\to i}^{(l-1)} A_i^1 + A_i^0} & \text{if } y_{i,b} = \neg x_i \\[2ex] \dfrac{i_{a\to i}^{(l-1)} A_i^0}{i_{a\to i}^{(l-1)} A_i^0 + A_i^1} & \text{if } y_{i,b} = x_i \end{cases}$$

Probabilistic interpretation:

$$\mathrm{Prob}(x_i) = \frac{A_i^0}{A_i^0 + A_i^1}$$

$$\mathrm{Prob}(\neg x_i) = \frac{A_i^1}{A_i^0 + A_i^1}$$

A BP-based decimation scheme consists in iteratively setting the variables with largest probability to be either true or false.

(This was probabilistic derivation as discussed and explained by Aurell, Gordon and Kirkpatrick in `cond-mat/0406217`).

To arrive at SP one introduces a modified system of beliefs, where every variable falls into one of three classes: TRUE in all solutions (1); FALSE in all solution (0); and TRUE in some and FALSE in other solutions (free).

A technique for exact computation of the partition function of $2D$ spin glasses.

A. Galluccio, J. Lukic, EM, O. C. Martin and G. Rinaldi, PRL 2004. Method from Galluccio, Löbl and Vondrák PRL 2000

Summary:

$Z_\beta^{ISG2D} \longrightarrow$ generating function of cuts

Galluccio-Löbl: it is possible to solve the Max Cut problem in polynomial time for any graph of genus bounded by a constant. The method provides directly the generating function of cuts.

$\longrightarrow$ Eulerian subgraphs

$\longrightarrow$ perfect matching

$\longrightarrow$ (on graphs of bounded genus) Pfaffian computation (square root of the determinant of an antisymmetric matrix). Need 4^g Pfaffians.

$\longrightarrow$ compute Pfaffian by using modular arithmetics (no need for infinite precision).

$\longrightarrow$ use the Chinese Remainder Theorem to reconstruct the exact partition function.

- Kasteleyn for planar graphs
  Galluccio-Löbl for graphs of bounded genus
  Perfect matching can be translated to a Pfaffian computation (of 4^g Pfaffian).

- Modular arithmetics. Work modulo some given prime number.
  Theorem: Let $P(x)$ be a polynomial of degree n with integer coefficients, $\Phi(p)$ a finite field of size $p > n$, and x_0, x_1, ... x_n distinct elements of $\Phi(p)$. Then there exists a unique polynomial of degree n over $\Phi(p)$ such that

  $$Q(x_i) = P(x_i) \bmod p, \quad i = 0, \ldots, n \ .$$

  The coefficients of $Q(x)$ are equal to the coefficients of $P(x)$ mod p.

- The Chinese Remainder Theorem.
  If we work in a number large enough of fields, i.e. p_1, p_2, ..., p_k such that

  $$\prod_{i=1}^{k} p_i > 2^n$$

  we can reconstruct the exact polynomial, i.e. the exact partition function. Great!

Summary of the Algorithm

1. Find prime numbers p_i such that

$$\prod_{i=1}^{k} p_i > 2^V \ .$$

   For each of them repeat steps 2, 3, 4 performing all operations in $\Phi(p_i)$.

2. Select $(m+1)$ distinct elements x_j of $\Phi(p_i)$. For each of them repeat step 3.

3. Write the 4^g matrices encoding the relevant orientations of the modified graph. This gives Z_β (in the point $e_\beta = x_j$).

4. From these values of $Z_\beta(\bmod p_i)$ in given points interpolate in $\Phi(p_i)$ and get the coefficients of the polynomial.

5. Apply the Chinese Remainder Theorem: compose the results from each $\Phi(p_i)$ to get the full Z_β.

Complexity: $O(V)$ finite fields, $O(V)$ evaluations in each field (for edge weights bounded by a constant), $O(V^{\frac{3}{2}})$ operations for a single evaluation of a polynomial $\Longrightarrow$ Total $O(V^{\frac{7}{2}})$.

J. Lukic, A. Galluccio, EM, O. Martin, G. Rinaldi.

$2D$ Ising Spin Glass, PBC, $J = \pm 1$.

For example:

L	S
6	400000
10	100000
30	10000
40	1000
50	300

(and similar values for different L values).

$$F_J(\beta) = -\frac{1}{\beta} \log Z_J(\beta) \quad , \; U_J(\beta) = \langle H_J \rangle \quad ,$$

$$c_V = L^{-2} \frac{dU_J}{dT} \quad ,$$

and average over samples. We mainly look at c_V (irrelevant constants are already subtracted).

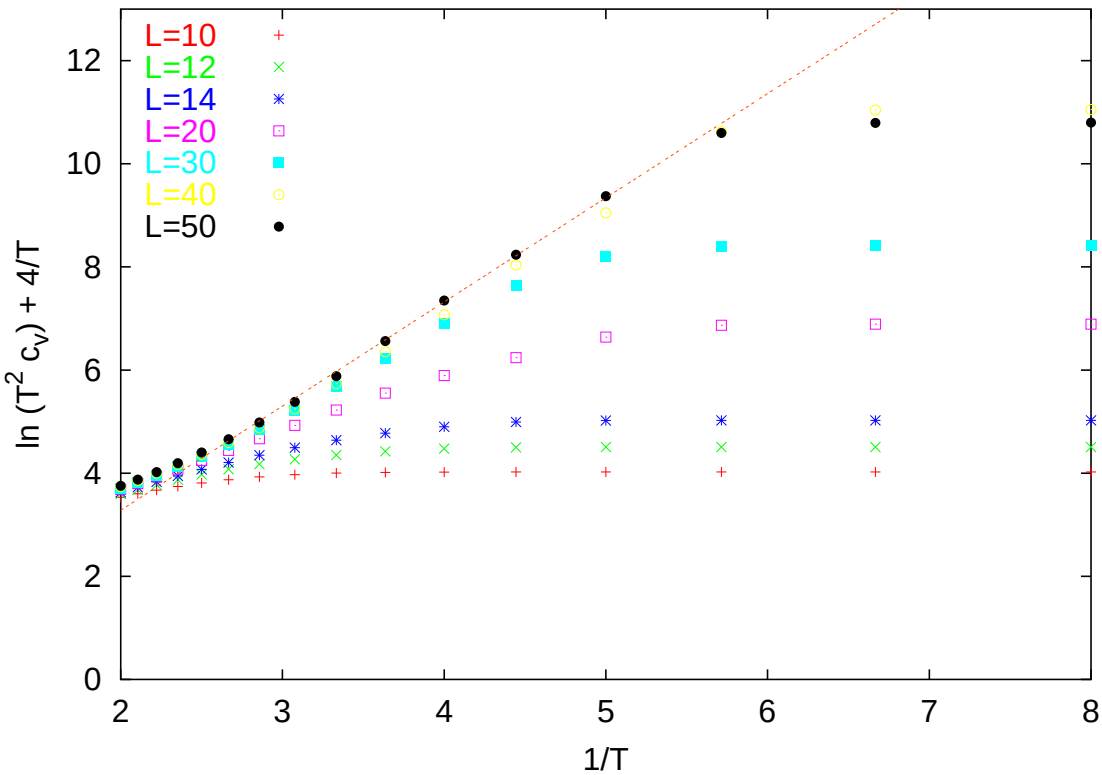
$$c_V \sim \beta^2 e^{-A\beta}$$

(we have checked that $p = 2$ is the best available choice for power corrections).

$$\log \frac{c_V}{\beta^2} \sim -A\beta$$

$$y \equiv \left(\log \frac{c_V}{\beta^2} + 4\beta \right) = (4 - A)\,\beta$$

So if we have naive scaling $y \sim$ constant in the scaling regime. If not: slope is $(4 - A)$.



Small T: saturation at constant value.

Intermediate T: $A \sim 2$.

Straight line: best fit $\beta \in [2.5, 5.5]$ gives $A = 2.02 \pm 0.03$.

Ultrametricity

I want to go back at last to ultrametricity, for sake of discussing a further technique (clustering).

Ultrametricity (UM) needs lot of space to emerge: it is really difficult to verify it on finite lattices.

Cacciuto, EM, Parisi 1996, Franz, Ricci-Tersenghi 1999.

Ultrametricity:

$$d_{13} \leq d_{12} + d_{23} \longrightarrow d_{13} \leq \max\left(d_{12}, d_{23}\right),$$

from triangular to (stronger) ultrametrical.

UM is an absolutely crucial feature of Parisi continuous RSB scheme. Consider two spin configurations α and β. Define a distance d from:

$$d^2_{\alpha,\beta} = \frac{1}{2}\left(1 - \frac{q_{\alpha,\beta}}{q_{EA}}\right)$$

equal to zero if $q = q_{EA}$, equal to 1 if $q = -q_{EA}$. Overlap:

$$q_{\alpha,\beta} = \frac{1}{V}\sum_{i=1}^{V} \sigma_i^\alpha \sigma_i^\beta \ .$$

Testing UM with Clustering

Clustering results of numerical simulations.

Domany, Hed, Hartmann, Stauffer 2001, Domany, Hed, Palassini, Young 2001.

We try to apply quantitative testing techniques Ciliberti, Marinari. We test MF: we know detecting UM is very difficult.

We find that the Z_2 symmetry has to be removed before any quantitative testing. This is very important: the ± 1 degeneracy completely obfuscates the results of the UM tests (see later).

Clustering (here for SK model with Gaussian couplings).

First you produce independent configurations (save $\forall$1000 full MC plus tempering sweeps) configurations at different (low) T values. N up to 512. T down to 0.2 (very low).

Set of configurations $\{C_t^{\tilde{T}}\}$. Compute overlaps at $T = \tilde{T}$ from $\sigma_{t'}^{\tilde{T}}(i)\sigma_{t''}^{\tilde{T}}(j)$, and since we are at equilibrium and configurations are uncorrelated this is a stationary sequence.

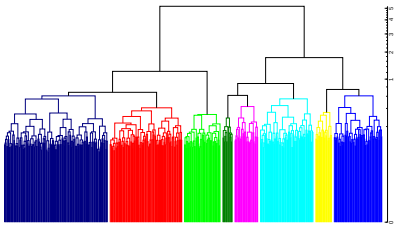
Clustering: partition data in "natural classes"':

- impose an ultrametric structure;
- check it it is natural.

Partition N objects into K clusters so that two points that belong to the same group are more similar than objects belonging to different groups.

Here we use, for the case $q \in (-1, +1)$ the definition $d \sim \frac{1-q}{2} \in (0, 1)$.

Hierarchical cluster algorithm $\longrightarrow$

dendogram.  There are many clustering algorithms one could use. Ward algorithm looks very suitable.

Fuse two clusters (individual objects are initial clusters).

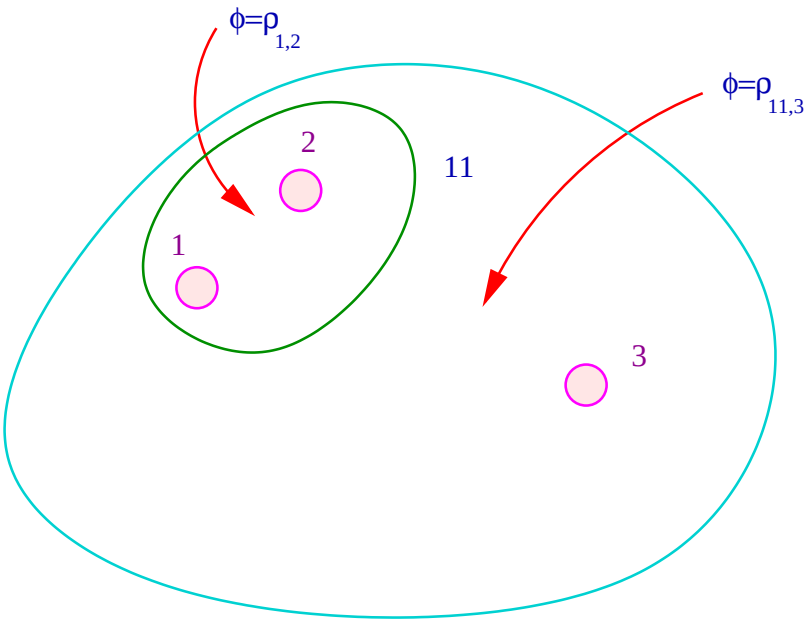
Initial partition: one object per cluster. Compute $D_{\alpha,\beta}$ among all "clusters". Fuse the two closer clusters:

$$\gamma = \text{“}\alpha \cup \beta''$$

Now define effective distance from this cluster to other clusters. For the process $\alpha + \beta \longrightarrow \gamma$, let n_α be the number of objects in cluster α. For all other cluster η we define $\mathcal{N} \equiv n_\alpha + n_\beta + n_\eta$. and

$$d_{\gamma\eta} = \frac{n_\alpha + n_\eta}{\mathcal{N}} d_{\alpha\eta} + \frac{n_\beta + n_\eta}{\mathcal{N}} d_{\beta\eta} - \frac{n_\eta}{\mathcal{N}} d_{\alpha\beta}$$

$$\phi(\gamma) \equiv d_{\alpha,\beta} \quad (\phi_{\text{initial configuration}}(\alpha) = 0)$$



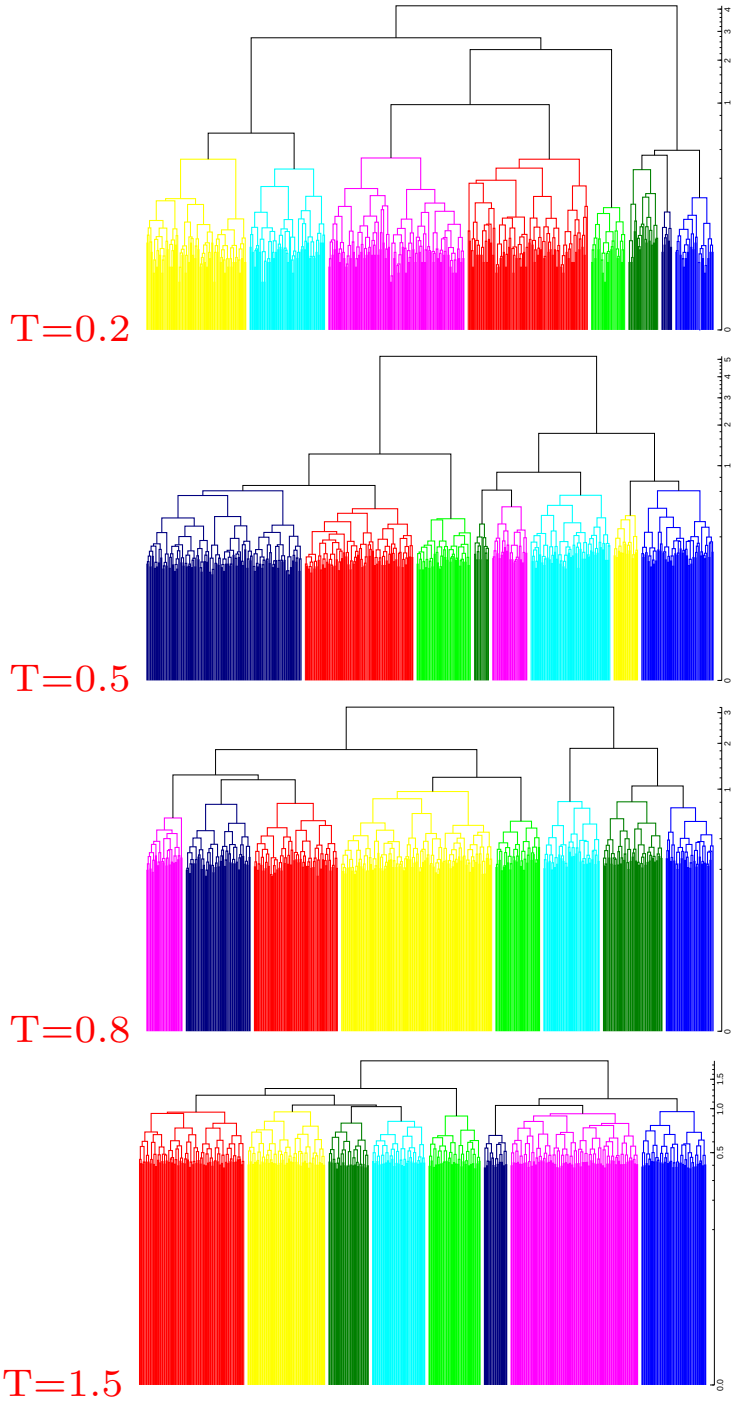
$$\delta(\gamma) = \sum_{\alpha,\beta\in\gamma} D^2_{\alpha,\beta}$$

distance of all couples of configurations in a cluster. Clusters formed earlier have lower ϕ and δ.

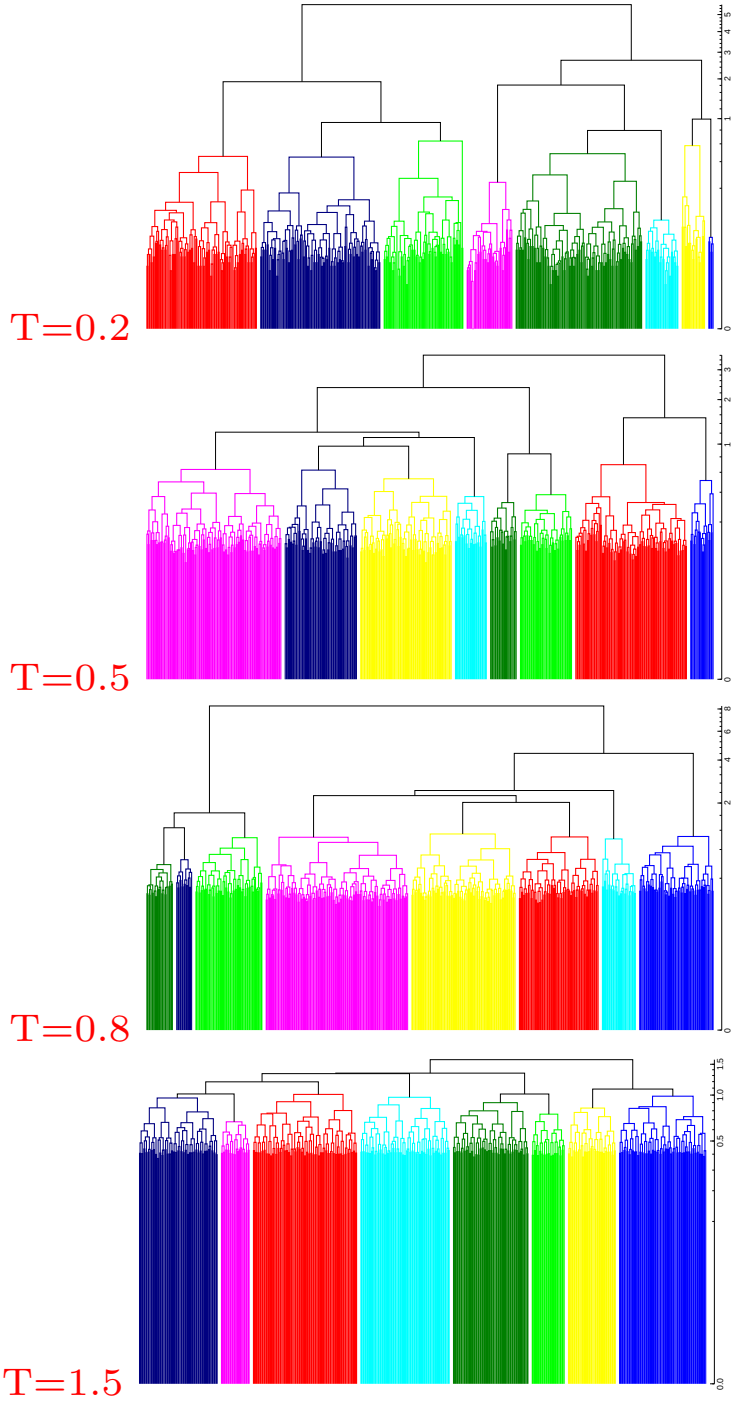
Output of the procedure is a dendogram. Leaves are configurations. Ascending the tree you coarsen. UM is built in.

Testing: are we detecting a real UM? A valid clustering is equivalent to the presence of an ultrametric structure. So, we have to check validity of the clustering.

Visual observation does not help much... (but scale is different).



A different disorder sample.



We summarize:

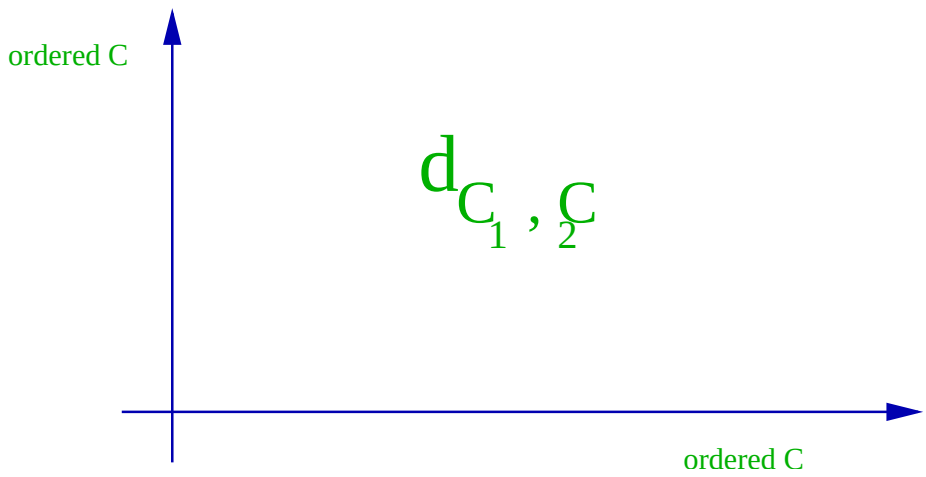
$$d_{\alpha,\beta} = \frac{1 - q_{\alpha,\beta}}{2}$$

by application of a cluster algorithm we obtain

a

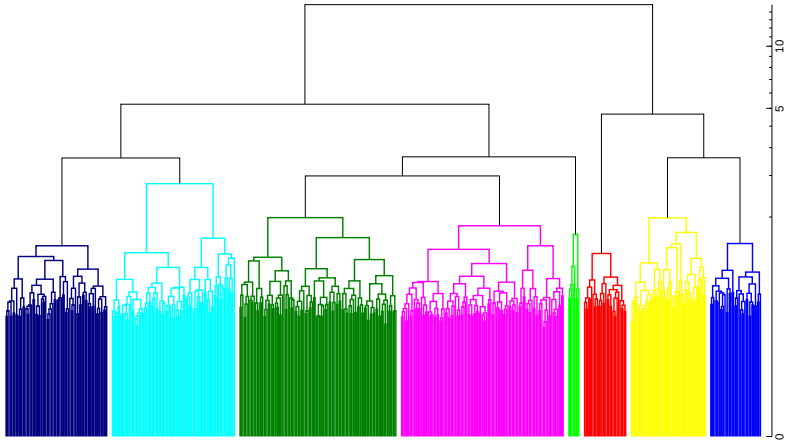
DENDOGRAM

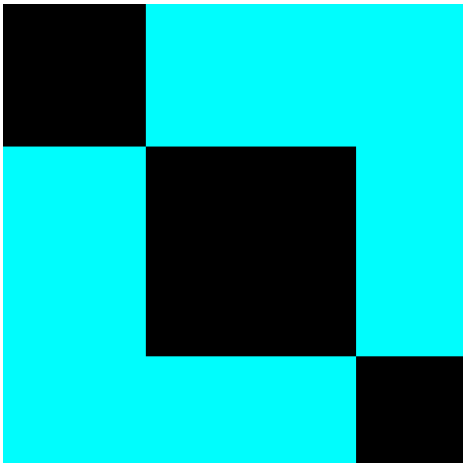
i.e. an ordering of the configurations enriched by a (cophenetic) distance

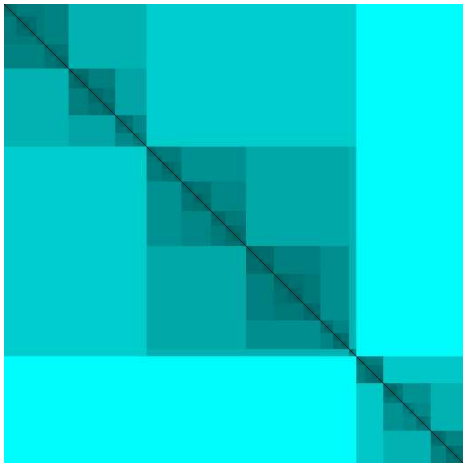


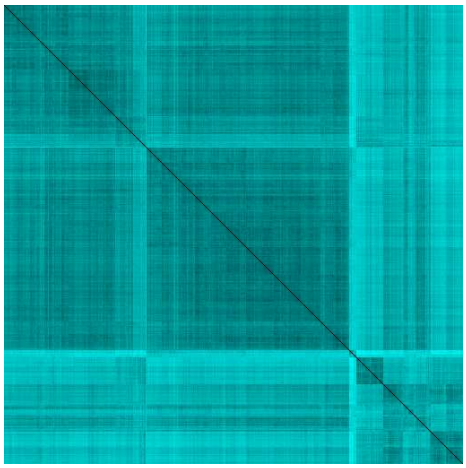
And now we can look at some figures.

SK, N=512, $T = T_c/2$



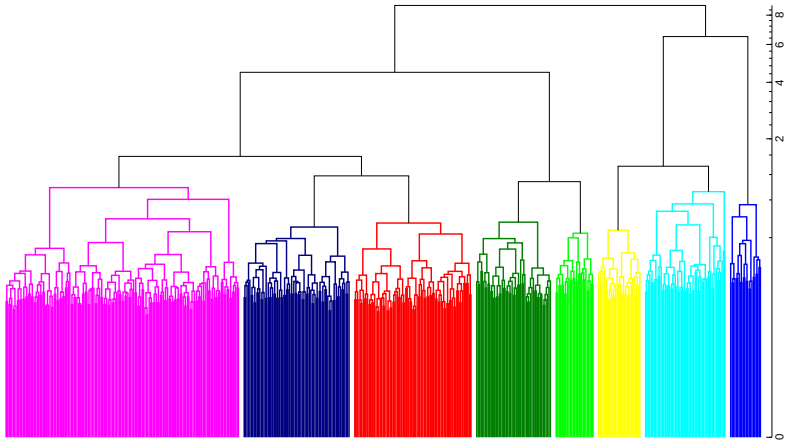


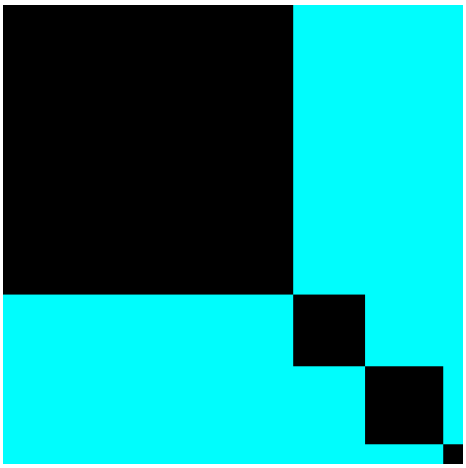


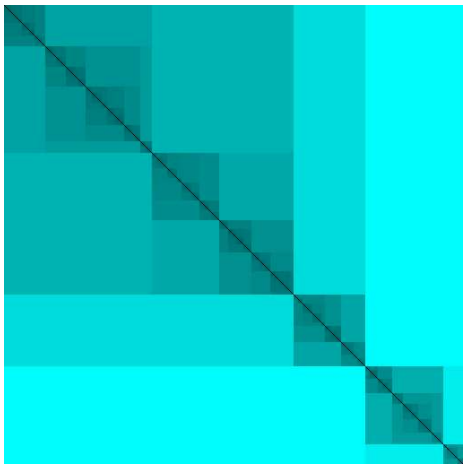


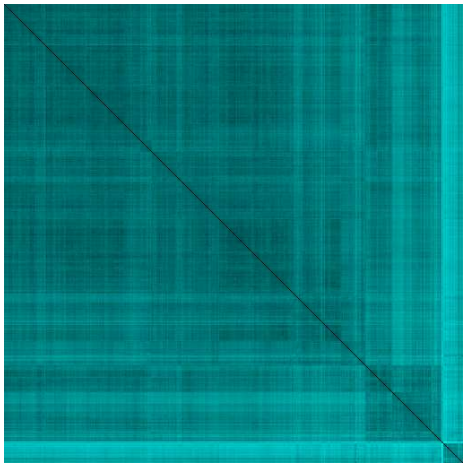
There is something good here.

SK, N=512, $T = T_c/2$









But much less here.

We discuss an important indicator, that tells us about the validity of the hierarchical structure.

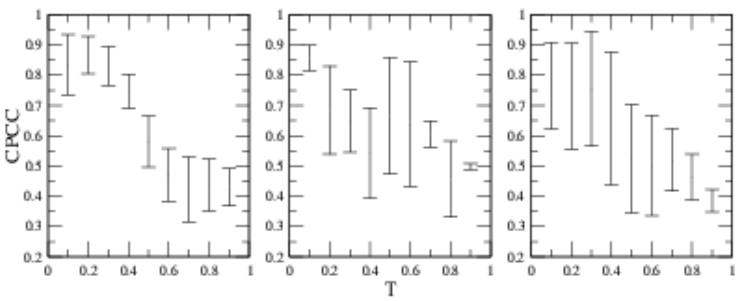
$d^C_{\alpha,\beta}$ cophenetic distance (UM by definition), i.e. the distance on the dendogram. $d_{\alpha,\beta}$ is the true distance.

$$\mathcal{K} \equiv \frac{\frac{1}{M^2}\sum_{\alpha,\beta} d^C_{\alpha,\beta} d_{\alpha,\beta} - \overline{d^C}\ \overline{d}}{\sigma_d \sigma_c}$$

It must be close to one to support the presence of a hierarchical structure (here there is not arbitrary threshold in the definition).

K is very used in numerical taxonomy. Empirically 0.9 is not enough (can establish accurately levels with MC as before).

Again, in presence of the Z_2 symmetry, K is very high and misleading. After removing it:



low, large errors, not very N dependent.

Detection on UM on "medium" size lattices is, even for MF models, very difficult or, better, impossible.