CURVED SURFACES, NON-PERTURBATIVE THERMODYNAMICS, & GLASSINESS

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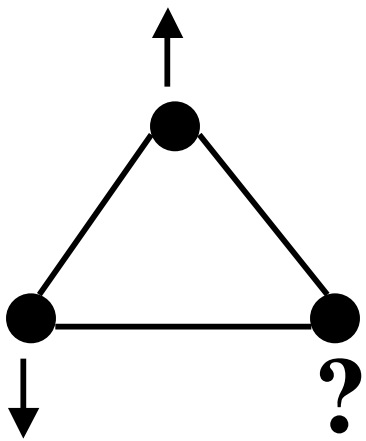
Conclusions

1. Geometrical constraints can lead to glassy dynamics and unusual thermodynamics. (Structural glasses)
2. By removing geometrical constraints, hard combinatorial problems whose simulated annealing dynamics are glass like may flow faster to their solution.

“Frustration”

Not all interactions can be simultaneously saturated



A classical example:

a triangular anti-ferromagnet

Geometrical Frustration in Glasses

- We will now study “non-Abelian” elastic analogs of constant external magnetic fields (which lead to Aharonov-Bohm phases and vortices in more conventional systems).

- In certain solvable limits, we find that these non-abelian backgrounds lead to slow dynamics and low ordering temperatures. The theoretical fits compare well with experiment.

Glasses: Physical Definition

- A glass = supercooled liquid (universal)
  Stupendous change in the relaxation times.

- False Urban Myth: The liquid-like character of glasses can be seen in old cathedrals (the windows are thicker at the bottom).

Glasses: Physical Question

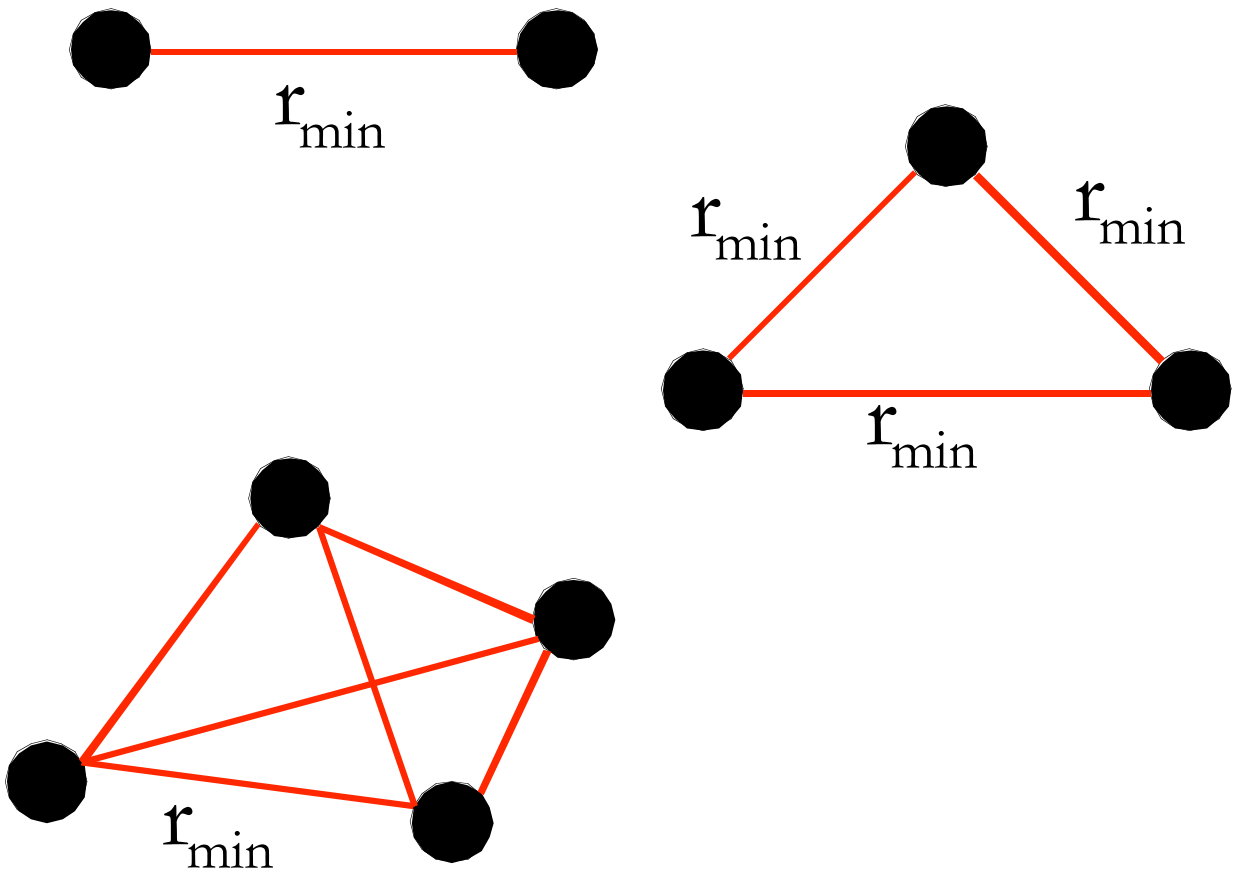
What sorts of configurations do we anticipate if we force the system to rapidly “compute’’ its low energy state?

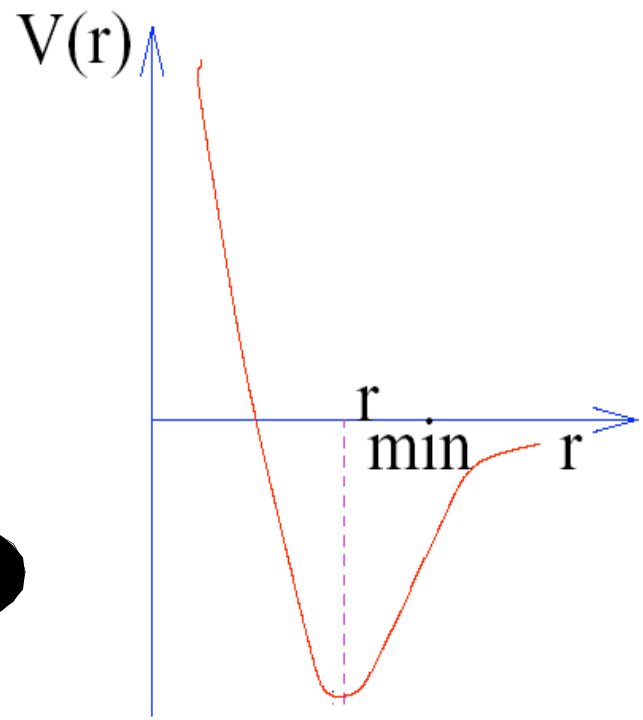
Glass Outline:

1. The notion of geometrical frustration in glasses
2. Gauge backgrounds
3. Deriving glassy dynamics in gauge backgrounds via replica calculations (new)
4. Non-perturbative thermodyanics: an avoided phase transition (new)
5. Comparing experimental fit parameters with theory (new)

I. Geometrical Frustration

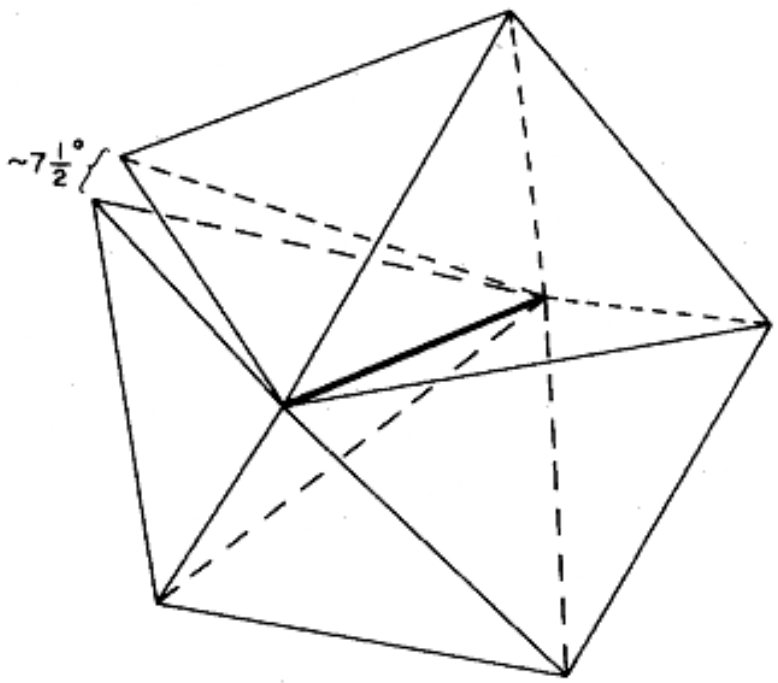
Ideal packing in a Lennard-Jones Liquid





We cannot keep going on forever

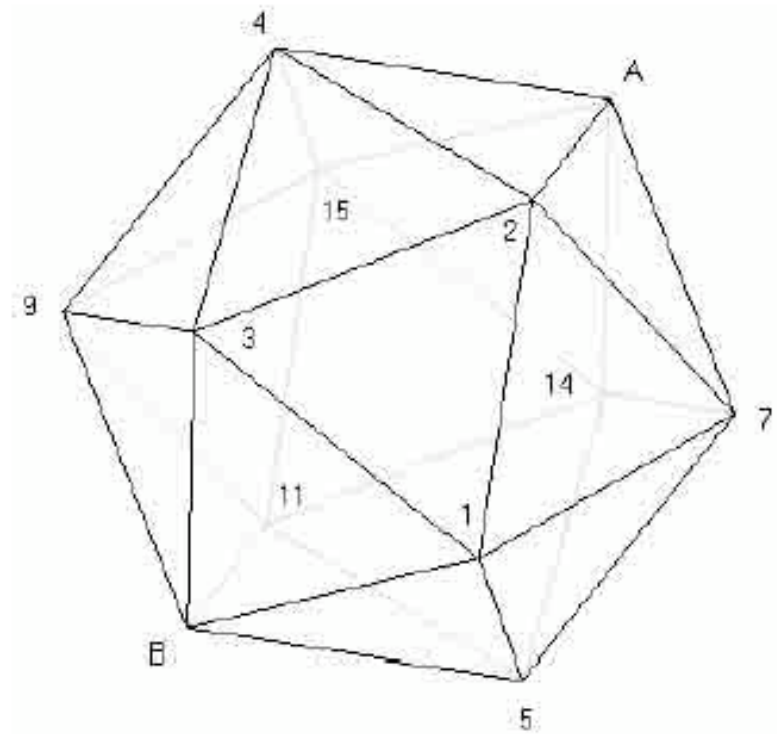
- The ideal packing can, however, be extended over a substantial volume if we consider the surface of a sphere embedded in d=4 dimensions.
- By endowing space with curvature we may remove the 7 degree void.



(J. Sethna, Phys. Rev. Lett. **51**, 2198 (1983))

An ideal configuration

Monte Carlo simulations show that 120 atoms cooled on the surface of a sphere find their ground state in a time less than 10^{-2} the time required to reach the fcc ground state in Euclidean space



Representation of the configuration (polytope {3,3,5})

(H. S. M. Coxeter, Regular Polytopes (1973))

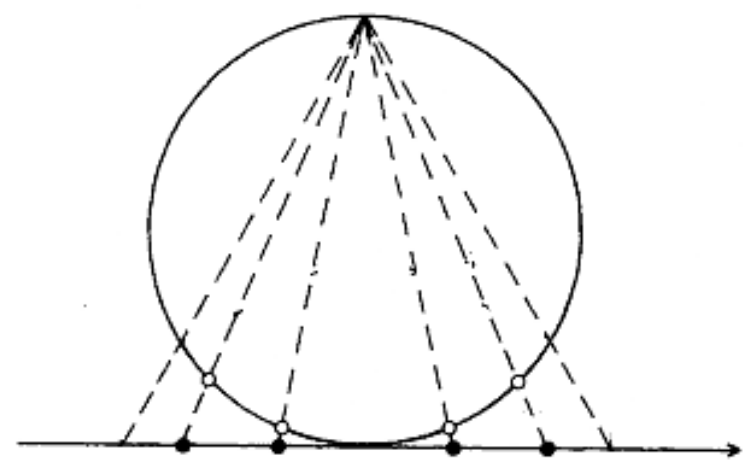
(J. P. Straley, Phys. Rev.B **34**, 405 (1986))

A viable working maxim

When a liquid is supercooled it may veer towards this or other local (high dimensional) minima before realizing that these configurations cannot tile space globally.

II. Gauge Backgrounds

Ideal template



Euclidean space x

These link the order on flat and curved space.

$$\rho_{\text{phys.}}(\vec{x}) = \rho(\vec{x}, \hat{u}_0)$$

$$\hat{u}_0 = (0,0,0,-1)$$

Project the particles onto the sphere

(S. Sachdev & D. R. Nelson, Phys. Rev. B **32**, 4592(1985))

$$\rho(\vec{x}, \hat{u}) = \sum_{n, m_a, m_b} Q_{n, m_a, m_b}(\vec{x}) Y_{n, m_a, m_b}(\hat{u})$$

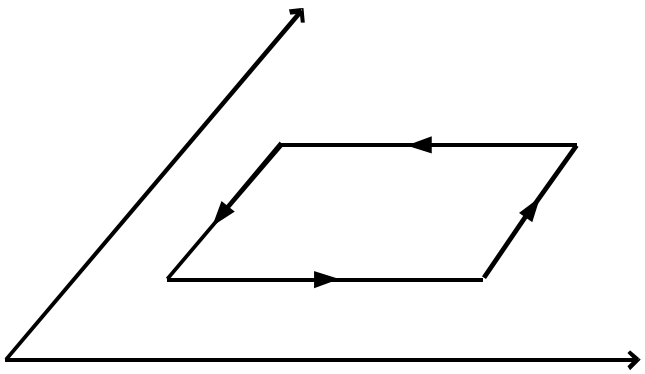
Landau-Ginzburg Expansion

$$F = \frac{1}{2}\sum_n (\kappa_n |D_\mu Q_n|^2 + r_n |Q_n|^2) + \ldots$$

$$D_\mu Q_n = (\partial_\mu - i\kappa L^n_{0\mu}) Q_n$$

The theory: that of a system subjected to a non-Abelian background (magnetic field) (S. Sachdev & D. R. Nelson, Phys. Rev. B **32**, 4592(1985))

A pictorial representation



$$Q_n(x)\big|_{final} = U Q_n(x)\big|_{initial}$$

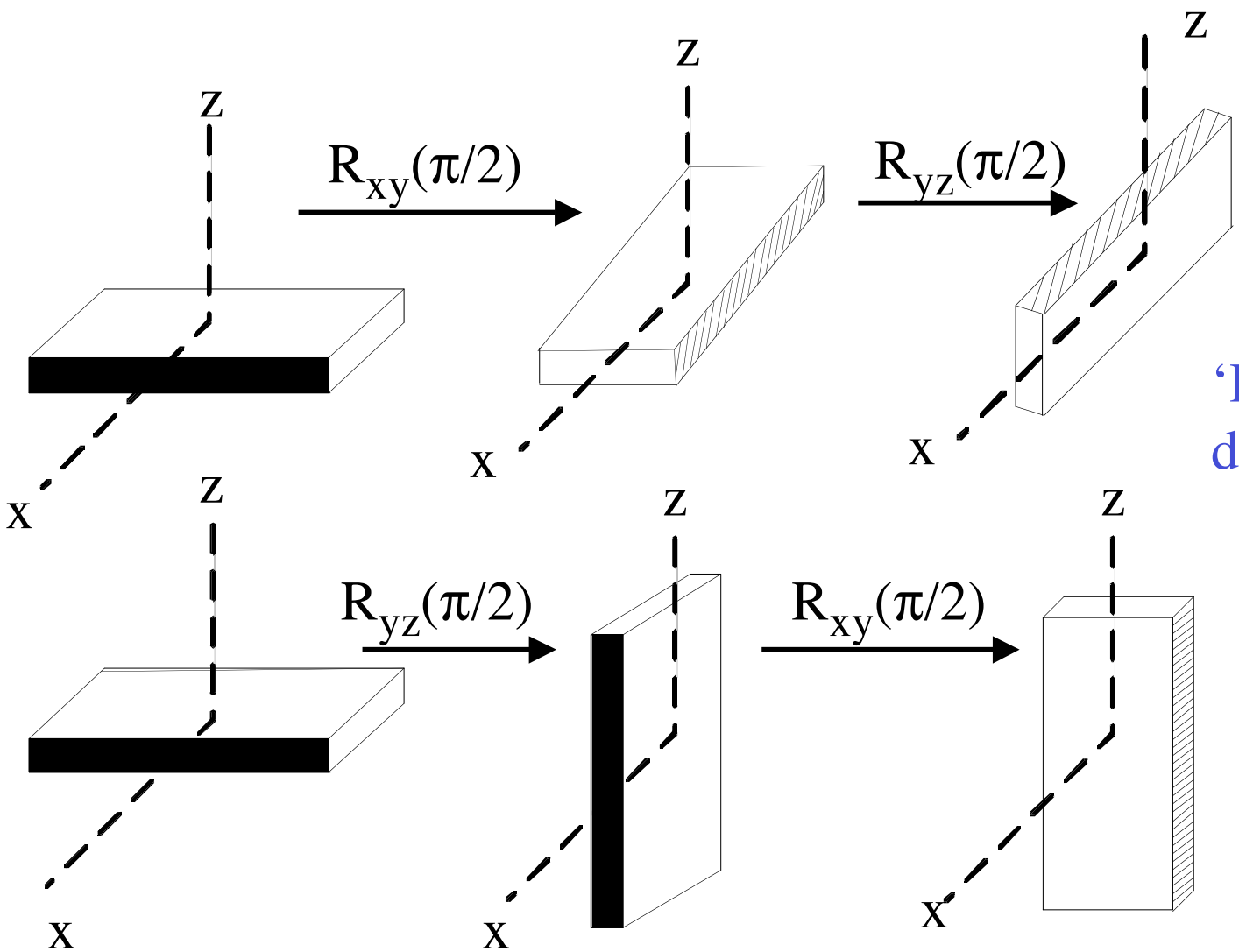
$$U \neq 1 \quad \text{as} \quad \left[L^n_{0\mu}, L^n_{0\nu}\right] = iL^n_{\mu\nu}$$

Ideal order
cannot prevail

The non-Abelian background gauge field creates frustration:

Non-Abelian Aharonov-Bohm phase

Non-commutativity of rotation generators



'Rolling' operators do not commute

$[R_{xy}, R_{yz}] \neq 0$

III. Glassy dynamics in geometrically frustrated systems (ZN, PRB 69, 014208 (2004))

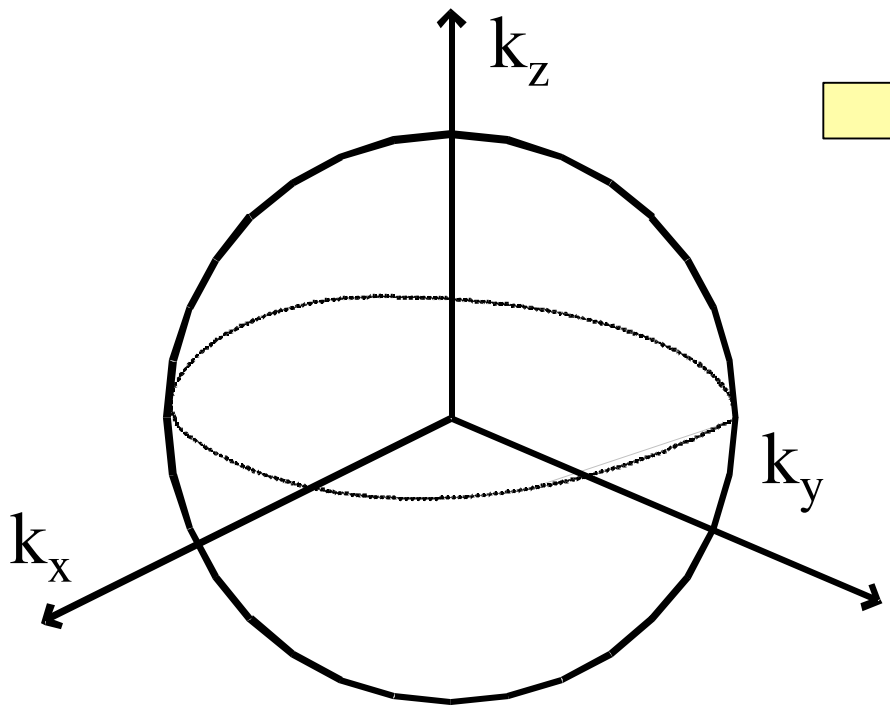
Geometric frustration leads to a multitude of degenerate and nearly degenerate states. This is easily seen in momentum space

$$F = \frac{1}{2} \sum_{n,i,\mu} \int \frac{d^3k}{(2\pi)^3} \, | \overset{\lambda}{\alpha}{}^{n}_{\mu,i}(\vec{k}) |^2 \, [\kappa_n \lambda^n_{\mu,i}(\vec{k}) + r_n]$$

By rotational symmetry of the energy, all eigenvalues $\lambda(|\vec{k}|)$

depend only on the magnitude of the wavenumber-
not its direction.

The minimizing manifold



As $k^{min} > 0$, ground states and metastable states proliferate

At low temperatures, only modes close to the minimizing manifold are important

$$G(k) \sim \frac{Z}{\xi^{-2} + (k^2 - q^2)^2}$$

The configurational entropy $S_c(T_K < T < T_A)$ is extensive

An exponential number of metastable states in non-abelian theories

Extensive configurational entropy

$$\Rightarrow \quad \tau \sim \exp[DT_K/(T-T_k)]$$

Glassy dynamics (Vogel-Fulcher)

This derivation may be repeated for any non-Abelian background. The dynamics on fixed curved surfaces is glassy.

Holographic ground state entropy

In this and many other related instances, we also proved that the ground state degeneracy is exponential in the surface area of system. Only modes on the minimizing manifold in momentum space are occupied:

$$\ln(g) \sim L^{d-1}$$

(links to a generalized Elitzur's theorem)

C. D. Batista, ZN (cond-mat/0410599), ZN & G. Ortiz, (cond-mat/0605316)

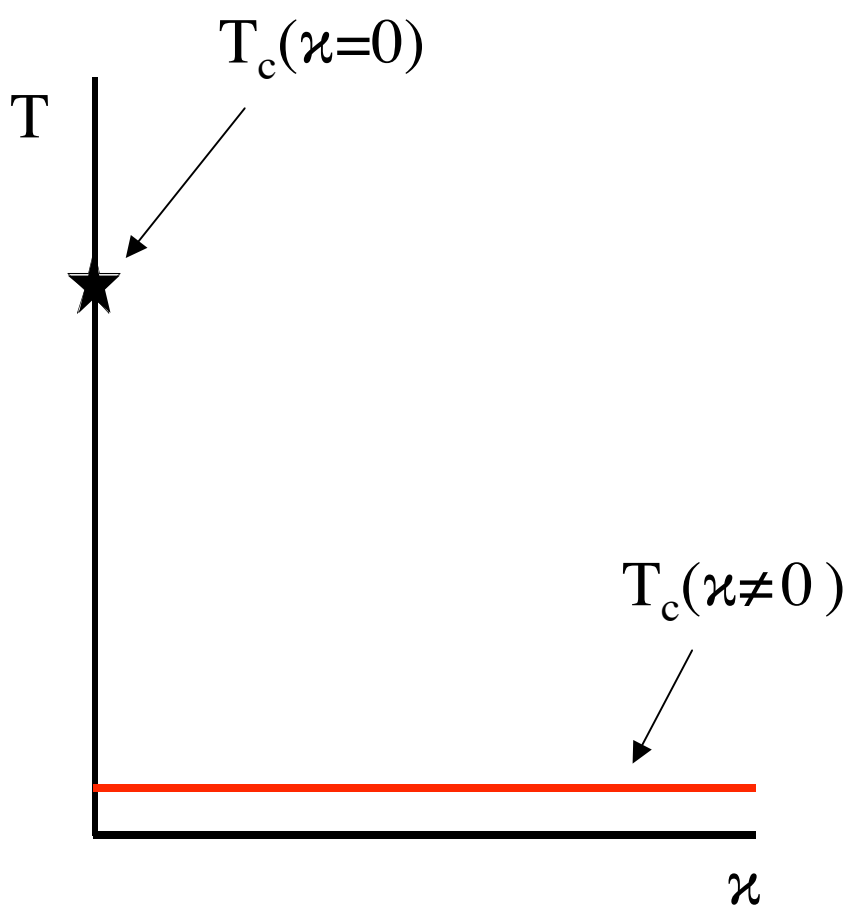
Unusual Equilibrium Thermodynamics: Avoided Phase Transitions

By performing a large n analysis (n=169 complex components in this theory) to second order in 1/n, deriving a generalized Mermin-Wagner theorem, and performing a thermal fluctuation analysis, we find that

$$T_c = 0$$

The thermodynamic phase transition is avoided!

The generic phase diagram



- For any finite curvature, the system is hot.
- Why is there no phase transition?
- The huge degeneracy and near degeneracy of the system makes it very susceptible to thermal fluctuations.
- All of this is true for all non-abelian fields.

Are there any empirically testable consequences?

Scaling away from the avoided critical temperature $T_c(\varkappa=0)$? Measurable quantities $F[(T-T_c(\varkappa=0))/T_c(\varkappa=0)]$?

V. Theory vs. experiment in the avoided critical fit for glasses

$$\tau = \tau_\infty \exp[E(T)/T]$$ relaxation time

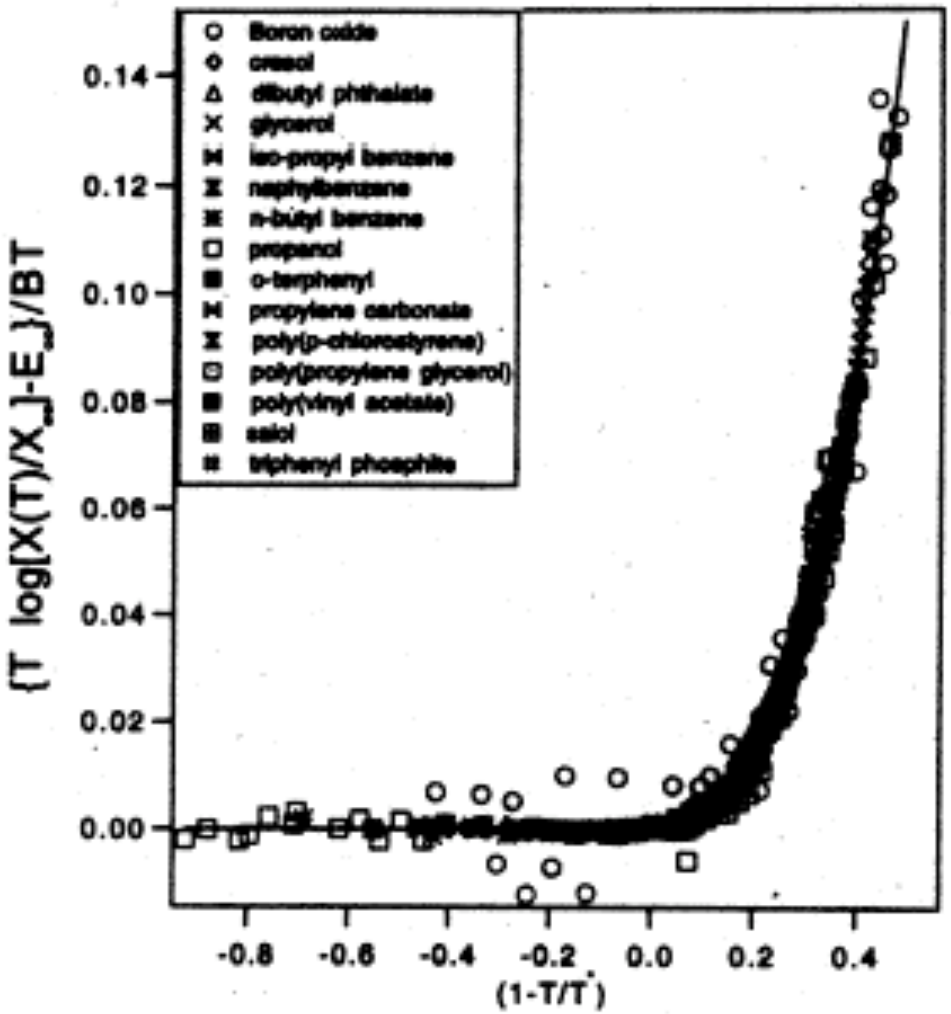
$$E(T) = E_\infty + (at)^{8/3}\theta(t)$$ free energy barrier

$$t = (T^* - T)/T^*$$ reduced temperature

$$T^* = T_c(\kappa = 0)$$ avoided critical temperature

Fit derived by domain wall energy considerations

An avoided critical fit



Works for all known glass formers.

(Physica A 219, 27 (1995))

A comparison between theory and experiment

glass former	$[T^{*}-T_{m}]/T_{m}$
n-butyl benzene	7.02%
triphenyl phosphite	8.2%
isopropyl benzene	20.6%
propylene carbonate	7.73%
sasol	-4.4%
dibutyl phthalate	21%
o-terphenyl	5.7%
s-trinaphthyl benzene	9.1%
n-propanol	30.6%
α-phenyl-cresol	-10.3%
glycerol	9.9%
glass former average	9.59%
Simple theory	8.4%

Simple theoretical analysis

$$\frac{E^{icosahedral} - E^{FCC}}{E^{FCC}} = 8.4\%$$

We expect T* to be indicative of the cohesive energy of the ideal curved space crystal and the natural melting temperature, T_{melt} to be correlated with the crystallization energy of the real crystal.

Conclusions
(new results)

- Geometrical constraints can lead to glassy dynamics and unusual thermodynamics.
- Phase transitions can be avoided.
- Possible relaxation time scaling with respect to the avoided critical temperature.
- An exponential number of ground and metastable states.

II. Dynamics in high dimensions

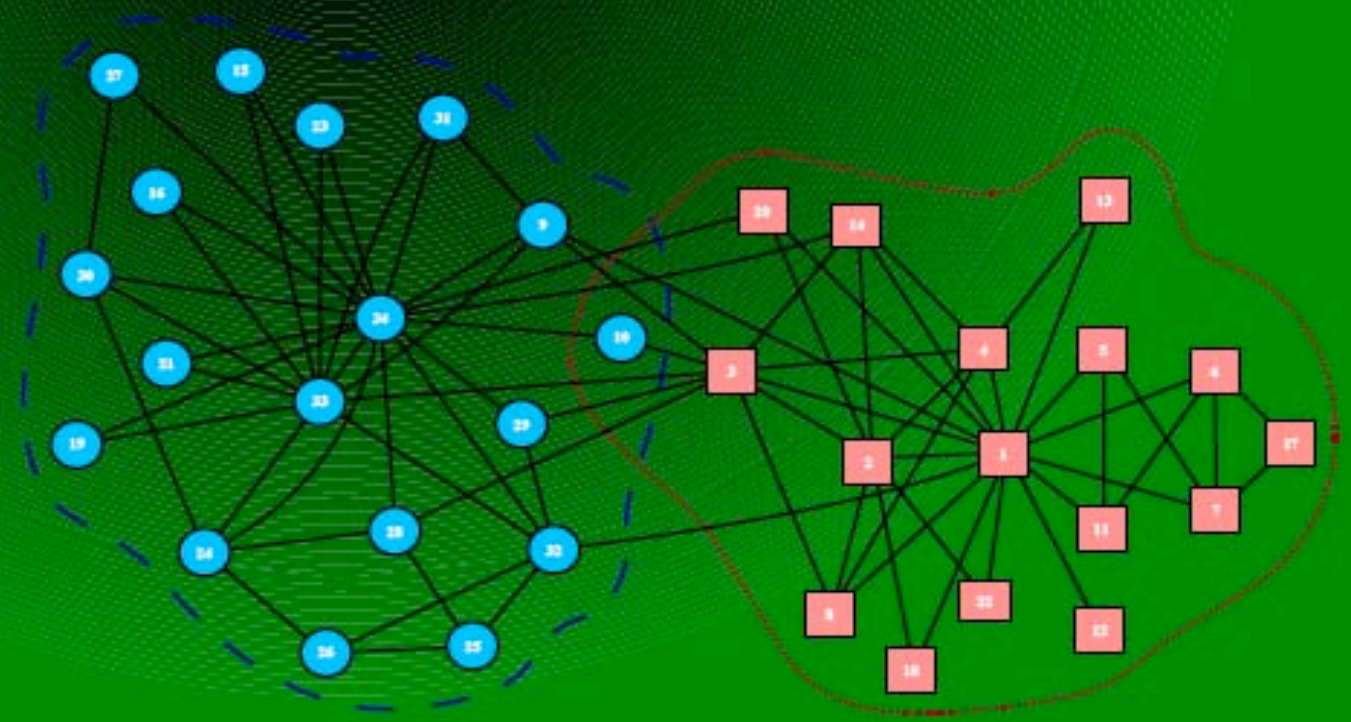
Outline (dynamics in high dimensions)

General idea

The largest clique problem

Community detection

Community Detection and Multi-Resolution Methods



Two approaches

- Dynamics in high dimensions can lead to the resolution of communities.
- A discretized Potts model (discrete dynamics in high dimensions)

Conclusions

(1) Approaches are free of the resolution limit problem and are able to determine the graph hierarchy

(2) Both are very accurate (Potts model as least as accurate as simulated annealing) and rapid.

Idea:

- By removing geometrical constraints, hard problems whose simulated annealing dynamics is glass like may flow faster to their solution. In high dimensions, there are fewer geometrical constraints.
- Less constrained systems -> faster dynamics. Can we make complicated calculations faster by increasing the dimensionality?

Application of the idea to the largest clique problem

P VS NP

The P versus NP Problem

Suppose that you are organizing housing accommodations for a group of four hundred university students. Space is limited and only one hundred of the students will receive places in the dormitory. To complicate matters, the Dean has provided you with a list of pairs of incompatible students, and requested that no pair from this list appear in your final choice. This is an example of what computer scientists call an NP-problem, since it is easy to check if a given choice of one hundred students proposed by a coworker is satisfactory (i.e., no pair from taken from your coworker's list also appears on the list from the Dean's office), however the task of generating such a list from scratch seems to be so hard as to be completely impractical. Indeed, the total number of ways of choosing one hundred students from the four hundred applicants is greater than the number of atoms in the known universe! Thus no future civilization could ever hope to build a supercomputer capable of solving the problem by brute force; that is, by checking every possible combination of 100 students. However, this apparent difficulty may only reflect the lack of ingenuity of your programmer. In fact, one of the outstanding problems in computer science is determining whether questions exist whose answer can be quickly checked, but which require an impossibly long time to solve by any direct procedure. Problems like the one listed above certainly seem to be of this kind, but so far no one has managed to prove that any of them really are so hard as they appear, i.e., that there really is no feasible way to generate an answer with the help of a computer. Stephen Cook and Leonid Levin formulated the P (i.e., easy to find) versus NP (i.e., easy to check) problem independently in 1971.

Lecture by Vijaya Ramachandran at UT.ram

Official Problem Description.pdf

A tale of a dean

The dean needs to place 100 out of 400 students in a dorm. So 1st come 1st …, or alphabetically, or poorest,

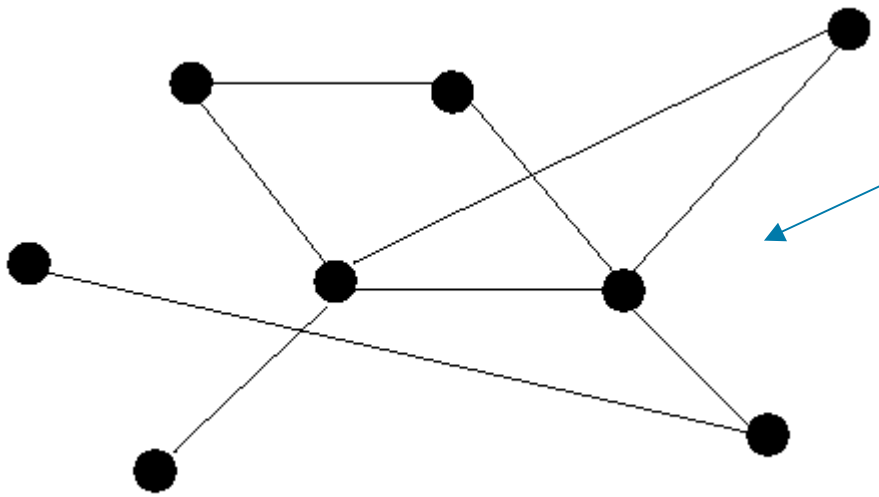
But all come with at the same time, all equally deserving, all start with J.

So lottery. But here comes:

Student #1 (John) comes with a big list of 170 students that he will never share a dorm with…

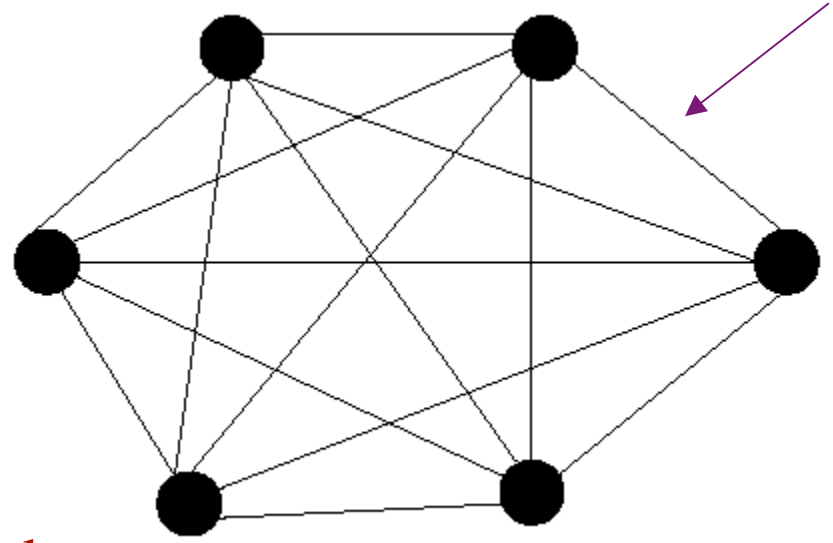
Student #400 comes with a big list if 260 incompatibles.

Graphical representations



Connect a line between students I and J if they are compatible.

A clique of 6 members



Look for a cluster (a "clique") within which each vertex is connected to all others.

The dean needs a clique of 100 students

A brute force approach

How to find the maximal set of compatibles?

Just put on the boots and go into the field.

Take Janine because she excluded the least number of students. However, the 250 that she likes are excluded by many. Taking John now at step 10^6 will exclude Jay 10^7 steps later.

There are, ab initio,

$$\binom{400}{100} \approx 2 \times 10^{96}$$ possible configurations.

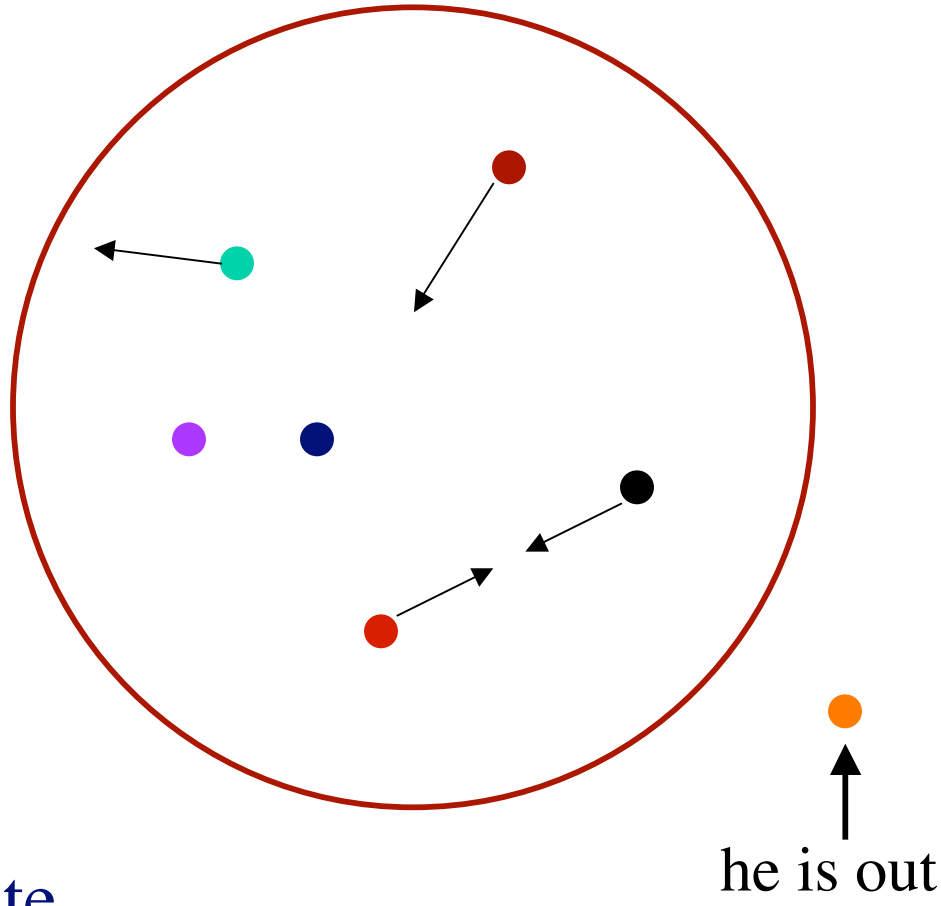
The thinking dean

A forceful physical approach

So the dean is desperate!

Then he has an inspiration.

Let them fight it out.

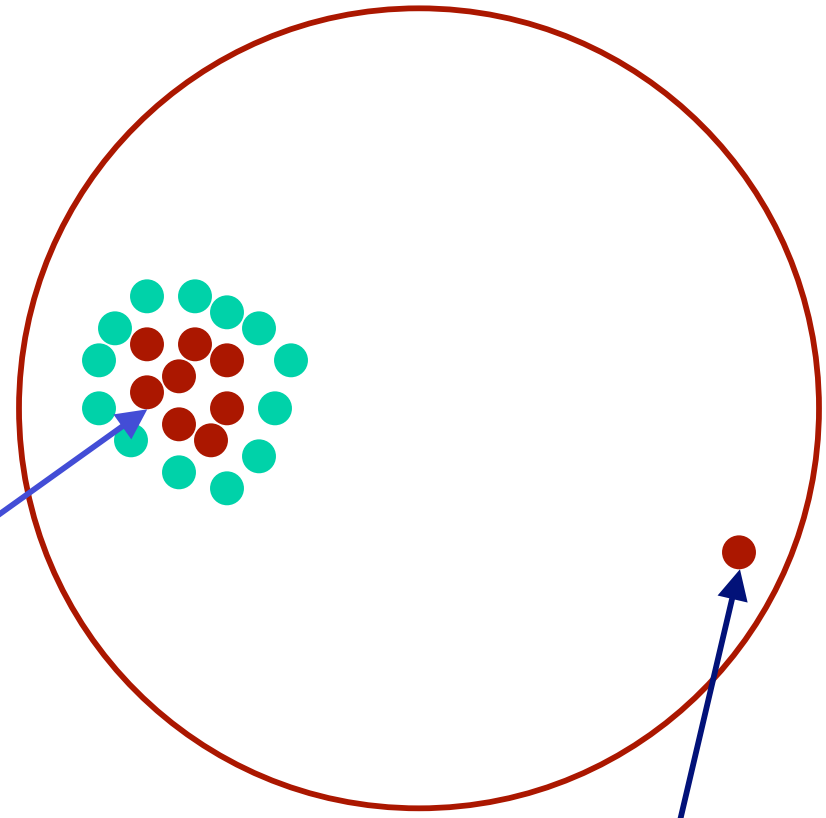


Pull in whoever you like

Push out whoever you hate

The failure of the forceful approach

Even if all the students are equally strong, the results are biased by initial placements and shielding, and will not be optimal.



good candidates surrounded by bad candidates and ejected with them

good candidate placed near the boundary and ejected early on

The ordeal of low dimensions.

What to do next?

At time t=0, we need to place the students symmetrically at

$$\vec{r}_i(0), \qquad i = 1,\ldots,N\ (=400)$$

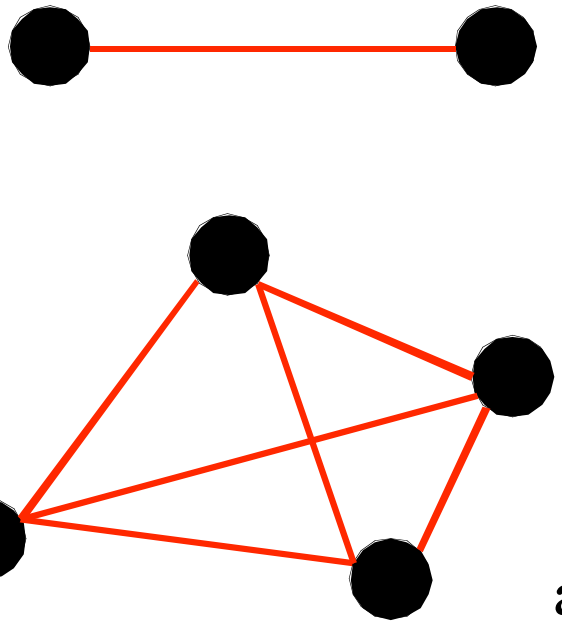
Such that for all $i \neq j$

$$|\vec{r}_i - \vec{r}_j| = \text{constant}$$

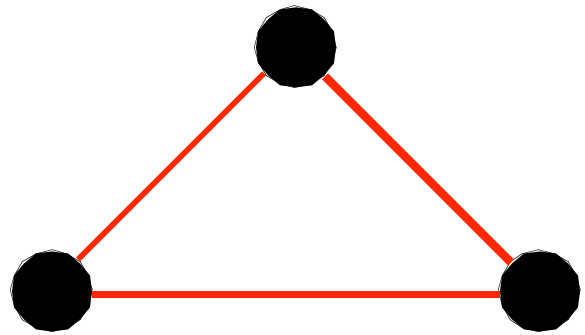
This can only be done on the vertices of a symmetric N-simplex in (N-1) dimensions!

The simplex at t=0:

2-simplex



4-simplex



3-simplex

and so on .

We encountered similar polytopes
in the glass problem

Why are high dimensions useful?

There is no shielding. Fewer metastable states. The number of vertices N=d+1, with d the dimension. No cancellation of force components can occur to produce bad ejections or undesired pulls. The faster dynamics towards more stable minima correspond to the distortion of a simplex in (N-1) dimensions.

Old lower dimensional worries: The formation of cliques may stop as any given point tries to move towards its designated clique, it might be overwhelmed by many repulsive forces which prevent it from joining the clique. Are there not many false minima which may trap the system- just as in the glass and spin-glass problems??

Intuitive argument for the absence of false minima

$$\sum_j \vec{F}_{j \to i} \neq 0$$

(N-1) independent vectors in (N-1) dimensions do not sum to zero (unless we collapse to a lower dimensional manifold)!

The vertices respond simultaneously to all forces.

All constraints imposed simultaneously.

Our physical system

$$U = \underbrace{\sum_{ij} C_{ij} \left| \vec{r}_i - \vec{r}_j \right|}_{\text{attraction}} + \underbrace{g \sum_{ij} (C_{ij} - 1) \left| \vec{r}_i - \vec{r}_j \right|}_{\text{repulsion}}$$

C_{ij} =1 if i is connected to j, and is 0 otherwise.

$$\vec{F} = -\vec{\nabla} U = \mu \vec{V}$$ Overdamped (Aristo.) dynamics

$$g \leq N - 1$$ (upper bound in collinear case)

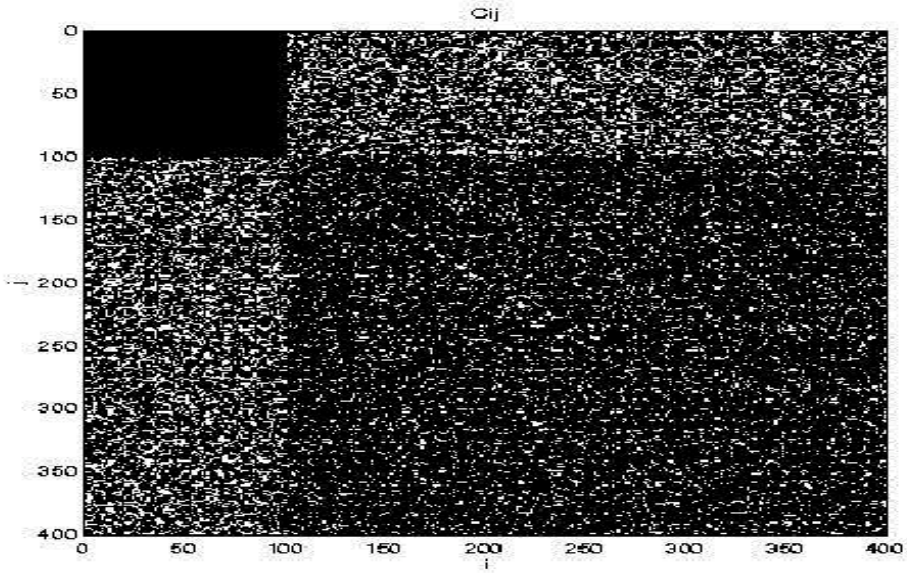
Good results already with g=2

Numerical results

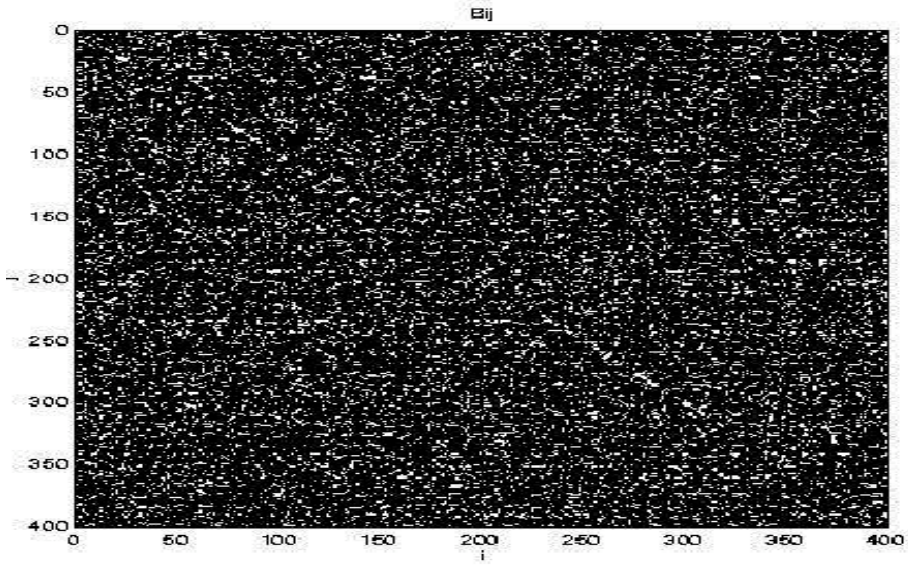
An example system consisted of an n=100 clique in an N=400 graph. Background valency is 90% for a partially overlapping 300 x 300 cluster. An average of 50% reconnections in the rest. We easily achieved Numerical reconstruction of the clique.

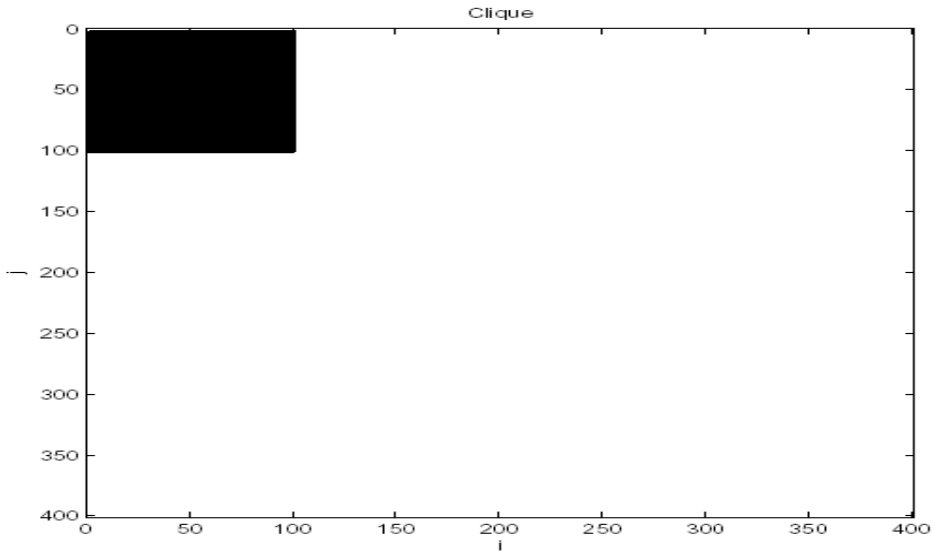
Numerical results

Original configuration



After permutation





g=2

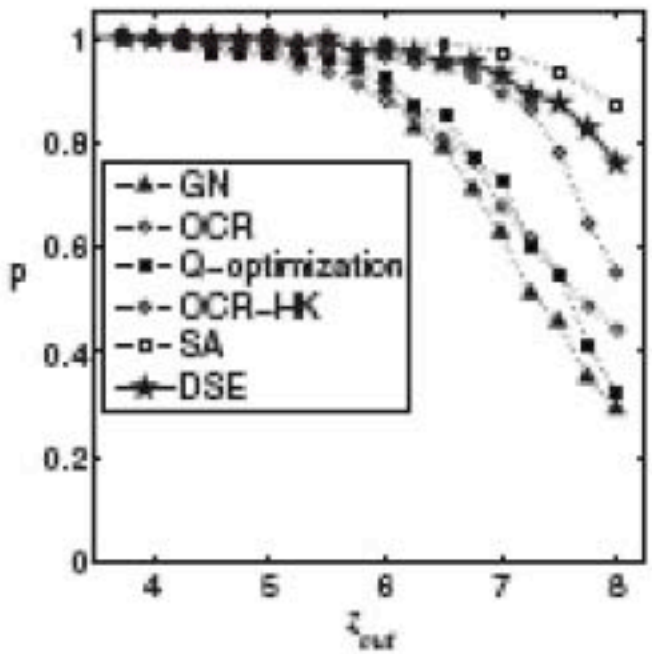
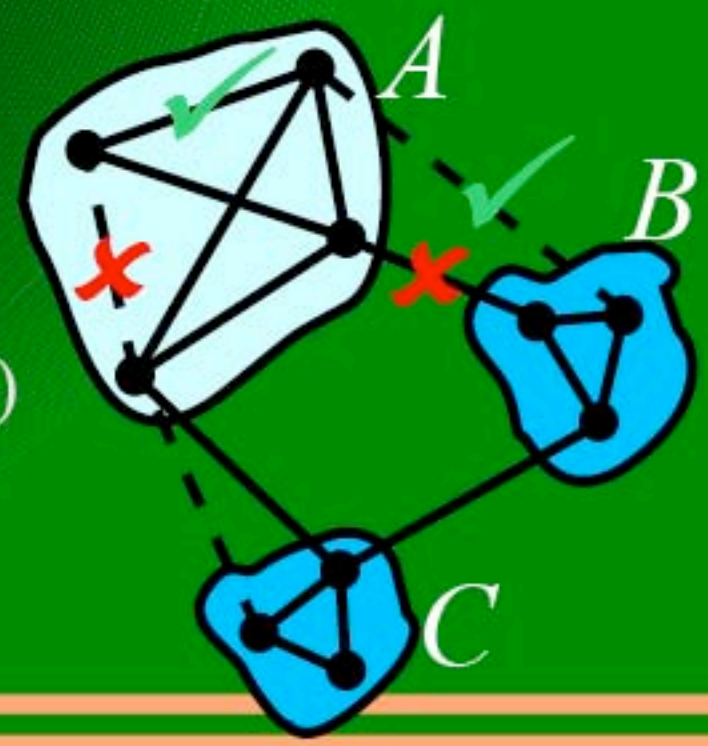


FIG. 3. Fraction p of correctly identified nodes as a function of z_{out} (average number of links between clusters per node) for computer generated random graphs with 128 nodes. The DSE algorithm is represented by stars, for the abbreviations of the other methods see [4].

Community Detection with a Potts Model

- Identify Nodes as Potts model spins
- Spin orientation $\sigma \leftrightarrow$ community assignment
  (with ferromagnetic *and* anti-ferromagnetic interactions)
- Energy Contributions
  - ✓ Inside Connected (–)
  - ✗ Inside Unconnected (+)
  - ✗ Outside Connected (+)
  - ✓ Outside Unconnected (–)



Community Detection with a Potts Model

- Optimal communities are found from the ground-state of a Potts Hamiltonian

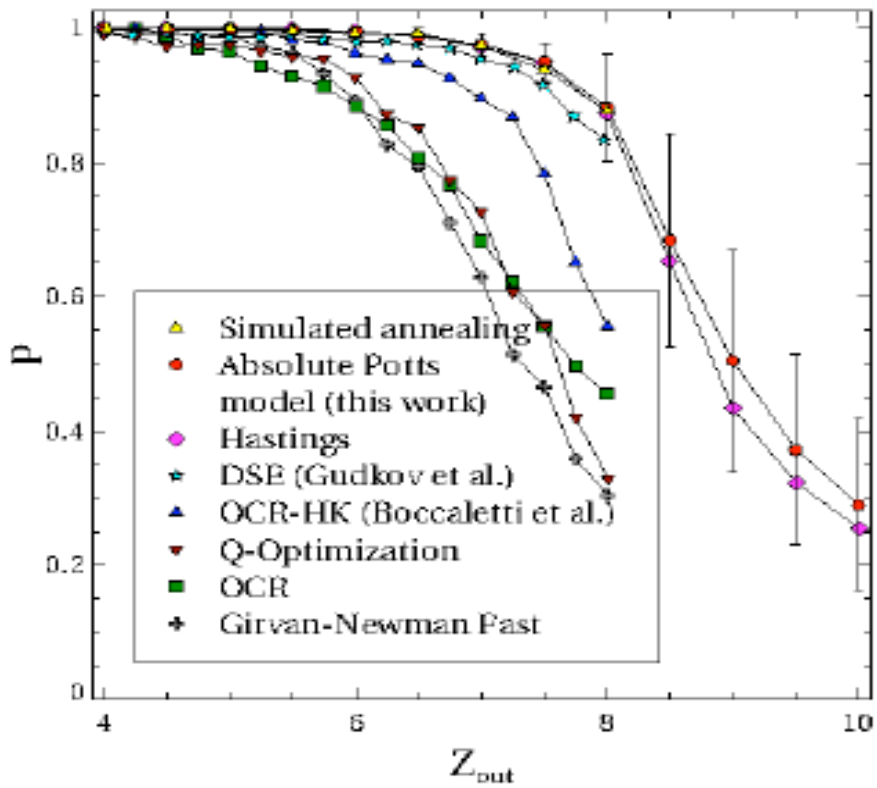
$$H(\{\sigma\}) = -\frac{1}{2}\sum_{i \neq j}(a_{ij}A_{ij} - b_{ij}J_{ij})\,\delta(\sigma_i, \sigma_j)$$

'good' contributions:
outside unconnected
inside connected

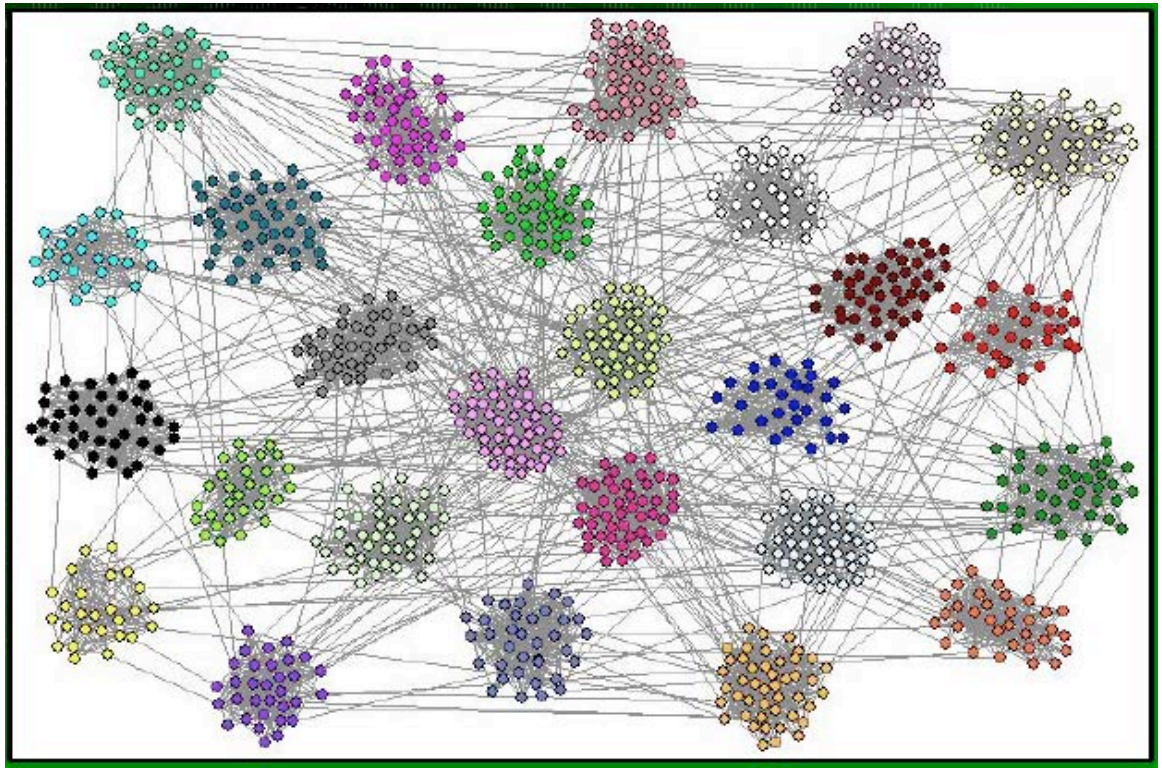
'bad' contributions:
outside connected
inside unconnected

- A_{ij} – the adjacency matrix, elements are 1 if nodes i and j are connected and 0 otherwise
- J_{ij} – the complement of the adjacency matrix, elements are 0 if nodes i and j are connected and 1 otherwise
- a_{ij} and b_{ij} are respective weights of the adjacency matrix elements and its complement

Numerical results

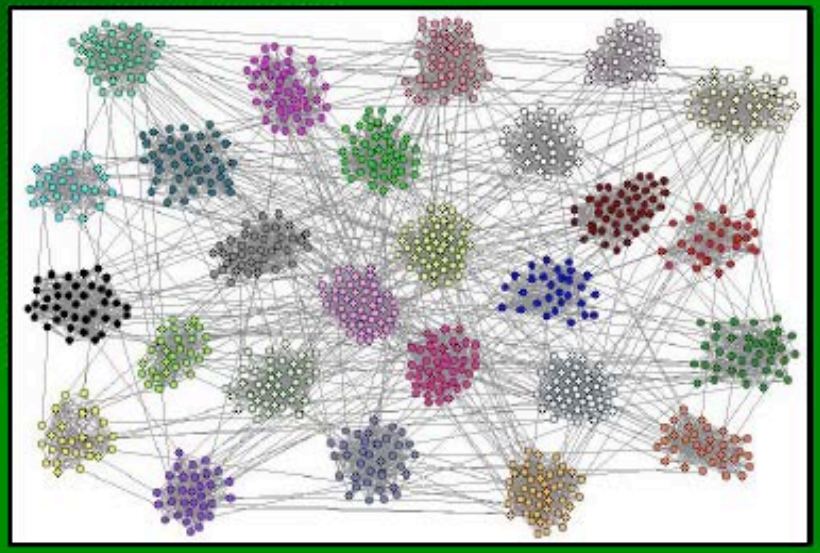


Lancichinetti-Fortunato-Radicchi benchmark

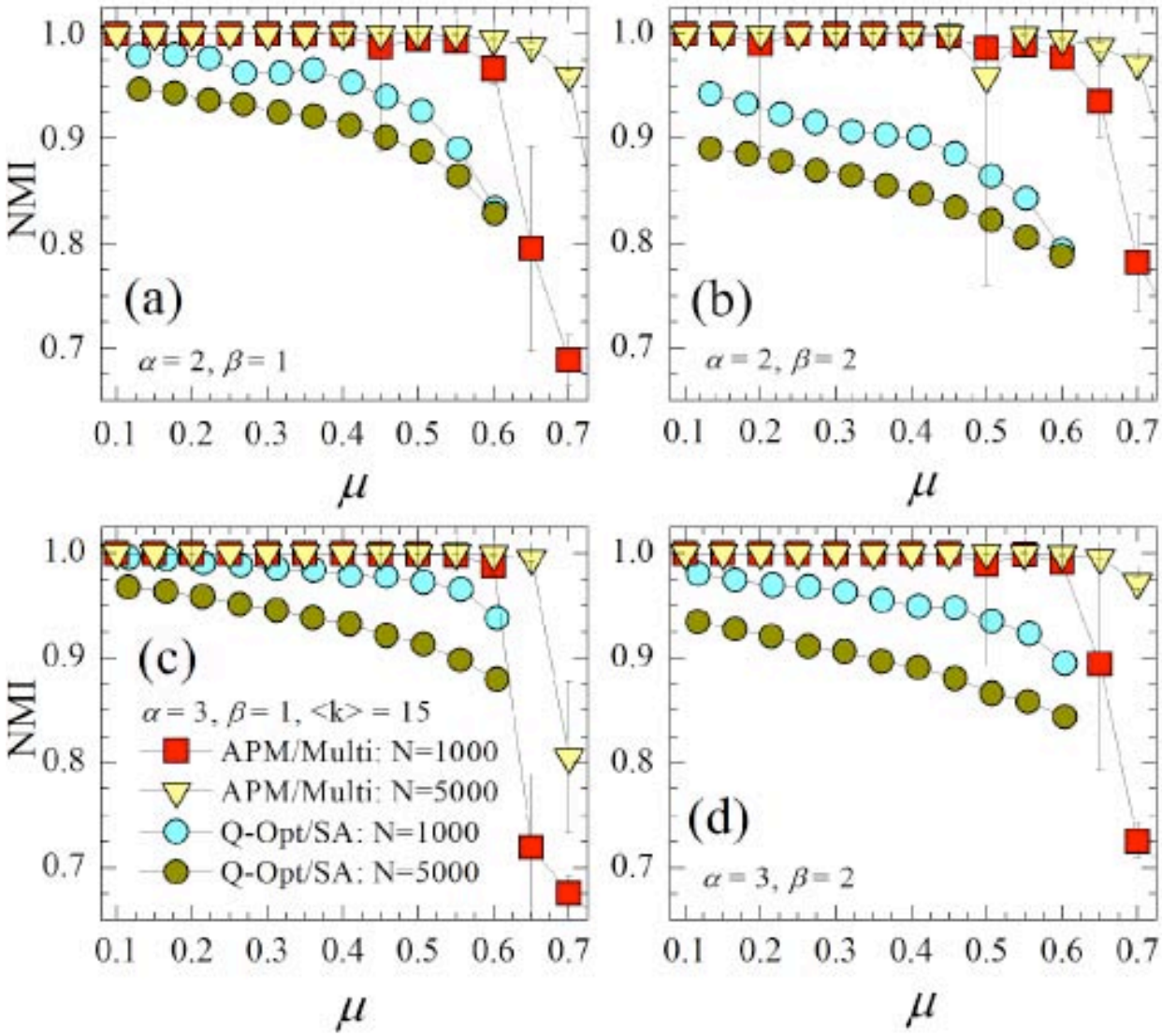


Multiresolution Accuracy: LFK Benchmark

- LFK benchmark features – a more "realistic" benchmark
  - Heterogeneous distribution of community sizes (power law with α exponent)
  - Heterogeneous distribution of node degrees (β)
  - Tests a large range of system sizes – N nodes
  - "Mixing parameter" μ – external degree fraction



Numerical results



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Community Detection with a Potts Model

- What is a resolution limit?
  - A popular quality function for community detection is modularity[1]

$$Q = \sum_{i=1}^{q} \left(\frac{l_i}{L} - \left(\frac{d_i}{2L} \right)^2 \right)$$

- q – the number of communities
- L – the number of total links in the system
- l_i – the number of links in community i
- d_i – the sum of the number of links in community i

Community Detection with a Potts Model

- Resolution limit: The effect is not drastic; but if a community division is solved by maximizing modularity, the number of communities q tends toward $\sqrt{L}$ where L is the number of links in the system[1–3,7]. The result is:
  - solution can merge smaller communities, or...
  - solution can divide large communities
  - *i.e.* the solution is affected by a global parameter of the graph that is being examined
- This Potts model eliminates these resolution limit issues[8]

Community Detection with a Potts Model

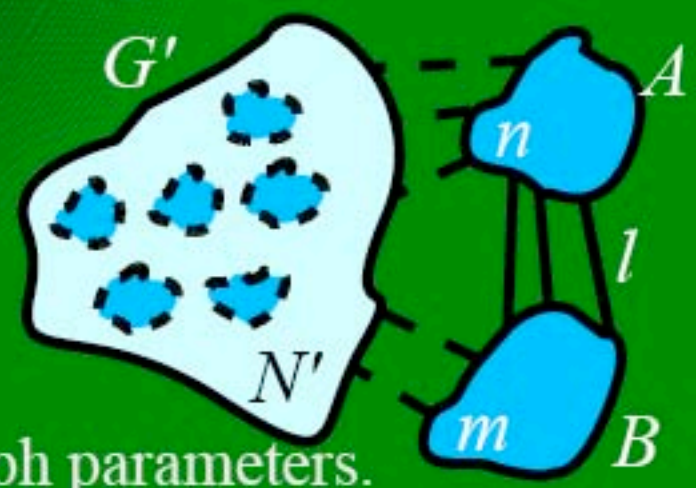
- Consider two communities A and B of size n and m connected by l edges in a graph G with N nodes.
  - modularity max. merges A and B (on average) if [2–4]

$$l = \frac{nm}{N}$$

  - Our Potts model merges them if [8]

$$l = \frac{\gamma}{\gamma + 1} nm$$

with no dependence on global graph parameters.



Community Detection Algorithm

- Select a desired weight γ in the Hamiltonian

$$H(\{\sigma\}) = -\frac{1}{2}\sum_{i \neq j}(a_{ij}A_{ij} - \gamma b_{ij}J_{ij})\delta_{\sigma_i\sigma_j}$$

γ determines a minimum density for communities.

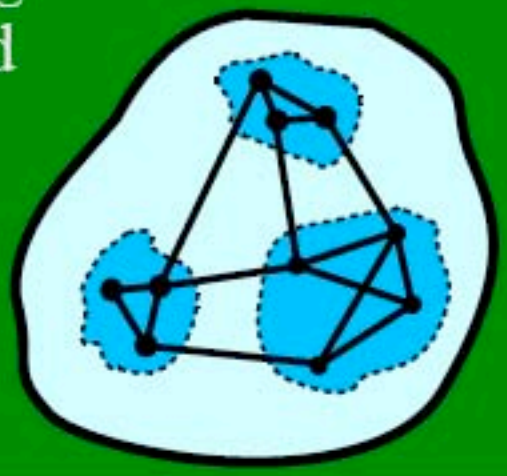
- Initialize the system to one node per cluster[10].
- Select a node sequentially:
  - Scan its neighbor nodes to determine the largest energy decrease (can be a new cluster). This is an $O(NZ \log Z)$ calculation for weighted graphs.
  - Move the selected node to that cluster if appropriate

Community Detection Algorithm

- Repeat above steps for all nodes
- Repeat all of the above steps until no lower energy moves are found.
- Repeat for a several configurations and select the lowest energy configuration as the solution.

Multi-Resolution Issues

- Systems can differ in optimal divisions based on the resolution at which the system is examined
  - Hierarchical systems
  - Unrelated multi-resolution structures
- Difficulty: Model does not 'scale' with system edge density or global graph parameters. 'Mixing' between divisions of a system is constrained by local parameters and an externally defined *graph-independent* global scaling.



Multi-Resolution Method

- Solution: Propose the following argument.
  - At the 'proper' resolutions of a system, different independent solutions should be more highly correlated
  - Conversely for 'in-between' resolutions, independent solutions will be less correlated due to 'mixing' occurring between competing divisions.
  - Other random effects will work to reduce the correlation between independent solutions

Normalized Mutual Information (NMI)

- Borrowed from Information Theory[6] and suggested for application in community detection
- $I(A,B)$ assesses how much 'mutual information' is present in two similar sets of data
  - $I(A,B) = 1$ if the two sets are perfectly correlated
  - $I(A,B) = 0$ if they are completely uncorrelated
- Start with a confusion matrix N_{ij} which indicates how many nodes of set A clusters are in each of the clusters of set B

Shannon Entropy

- Probability $P(k)$ that a random node will belong to community k

$$P(k)=\frac{n_k}{N}$$

n_k is the number of nodes in community k

N is the total number of nodes.

- Entropy of $P(k)$ for a partition A is

$$H(A)=-\sum_{i=1}^{q_A} P(k)\log P(k)$$

Mutual Information

- $I(A,B)$ is the Mutual Information (unnormalized)

$$I(A,B) = \sum_{i=1}^{q_A} \sum_{j=1}^{q_B} \frac{N_{ij}}{N} \log\left(\frac{N_{ij} N}{n_i n_j}\right)$$

  - Confusion matrix N_{ij} indicates how many nodes of cluster i in partition A are in cluster j of partition B
  - q_A and q_B are the number of clusters in partitions A and B

Information Measures: NMI and VI

- Normalized Mutual Information is

$$NMI(A,B)=\frac{2I(A,B)}{H(A)+H(B)}.$$

- Variation of Information is

$$VI(A,B)=H(A)+H(B)-2I(A,B).$$

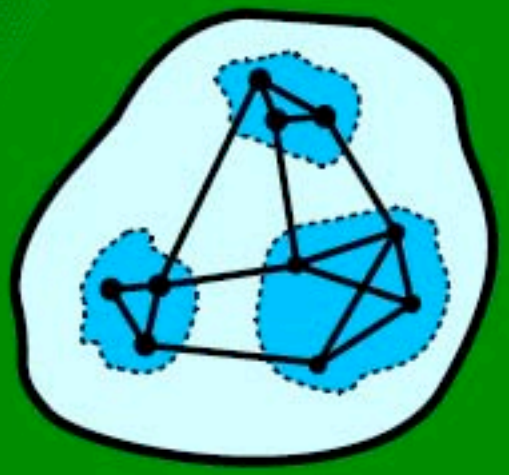
Normalized Mutual information

$$I(A,B)=\frac{-2\sum_{i=1}^{c_A}\sum_{j=1}^{c_B}N_{ij}\log\left(N_{ij}N/N_{i.}N_{.j}\right)}{\sum_{i=1}^{c_A}N_{i.}\log\left(N_{i.}/N\right)\sum_{j=1}^{c_B}N_{.j}\log\left(N_{.j}/N\right)}$$

- c_A and c_B are the number of clusters in sets A and B
- rows i are the clusters of set A
- columns j are the clusters of set B
- $N_{i.}$ – the sum of all j columns for row i
- $N_{.j}$ – the sum of all i rows for column j

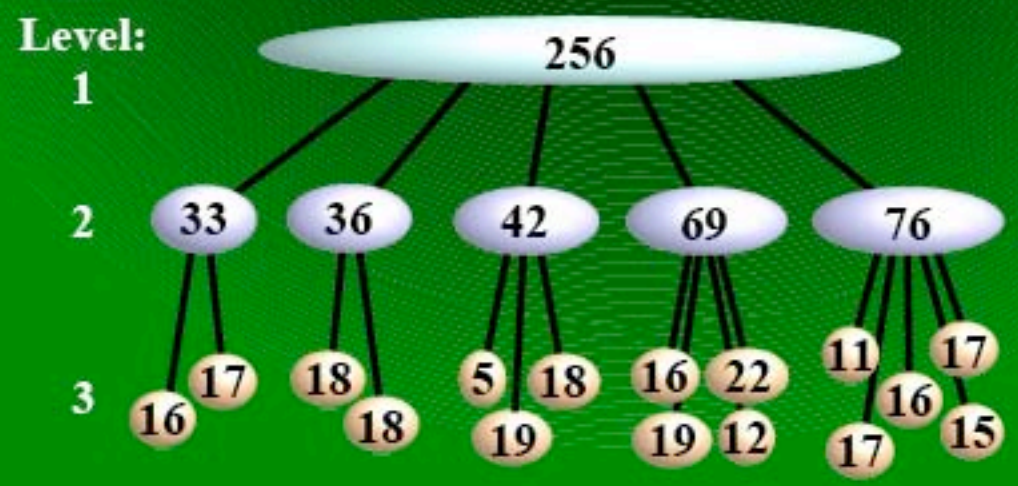
Multiresolution Systems

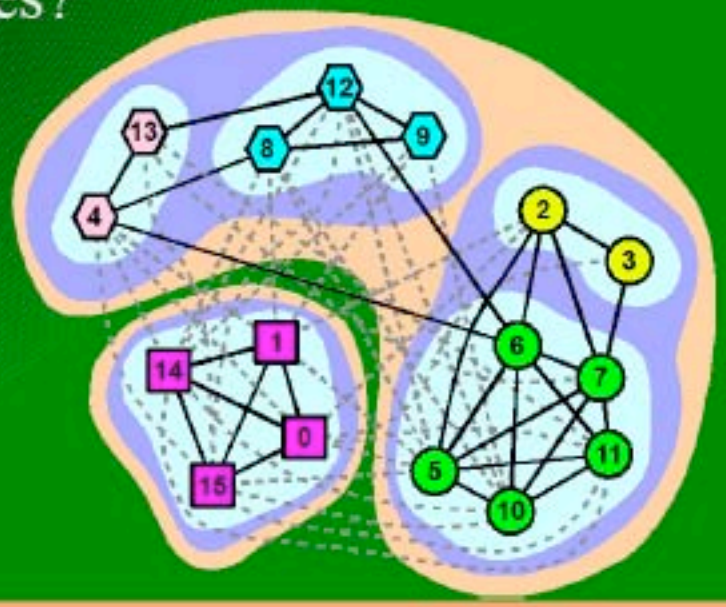
- Systems can differ in optimal divisions based on the scale at which the system is examined
  - Example: Personal relationships
    - Family
    - Close friends
    - Friends
    - Acquaintances



Multiresolution Systems

- Types of multiresolution structure:
  - Hierarchical
  - Overlapping structures
    (nodes shift membership at different scales)
  - Other multiresolution structures?





Multi-Resolution Method

- Examine a system over a range of resolutions by varying the edge weight γ for the model.

$$H(\{\sigma\}) = -\frac{1}{2}\sum_{i \neq j}(A_{ij} - \gamma J_{ij})\delta_{\sigma_i \sigma_j}$$

Or for a weighted system

$$H(\{\sigma\}) = -\frac{1}{2}\sum_{i \neq j}(a_{ij} A_{ij} - \gamma b_{ij} J_{ij})\delta_{\sigma_i \sigma_j}$$

- Determine the correlation between all pairs of solutions (at the same γ) via NMI.

Multi-Resolution Method

- Peaks in the NMI define the 'best' resolutions
- Peak values of the NMI give a quantitative estimate of the 'strength' of each division

Multi-Resolution Method

- Solution: Propose the following argument
  - At the 'best' resolutions of a system, independent solutions ("replicas") should be strongly correlated
  - For 'in-between' resolutions, independent replicas will be more weakly correlated due to 'mixing' between competing divisions.
  - Other random effects will work to reduce the correlation between independent solutions

Multi-Resolution Algorithm

- Solve the system several times to provide enough averaging for the solution correlations, $O(NZ \log Z)$ per solution since it is the base community detection method.
- Test each solution for local minima.
  - The energy landscape can trap the solution.
  - Although, some local minima actually carry useful information.
- Merge clusters as appropriate in order of largest energy decrease. It is $O(q^2)$ per merge for sparse systems due to the construction and analysis of a qxq energy matrix.
  - We merge all communities that lower the energy.

Multi-Resolution Algorithm

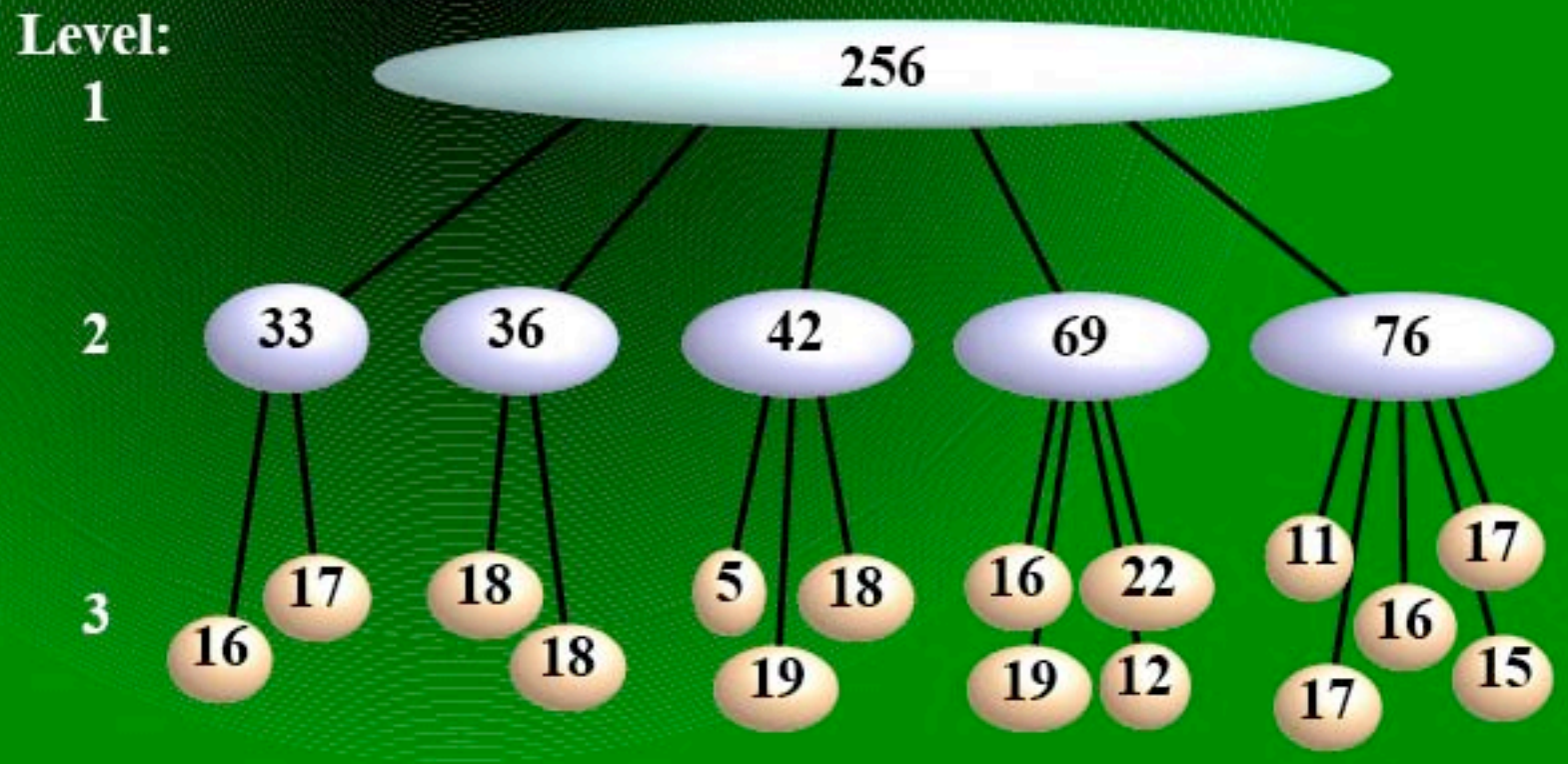
- Calculate the NMI between the all pairs of solutions, $O(q^2)$ per calculation for sparse systems due to building and analysis of the confusion matrix.
- Increment the edge weight γ and repeat above steps
- For each weight γ, plot the average NMI versus γ
- Find maxima in the NMI plot. These maxima will correspond to the multi-resolution structure(s).

Multi-Resolution Test System: Hierarchical

- Test system is a heterogeneous 3-level hierarchy
  - Level 1: 256 nodes with a random density of 0.1
  - Level 2: 5 groups with size ranging from 34 to 81 with an edge density of 0.3 each
  - Level 3: 16 groups with size ranging from 7 to 24 with an edge density of 0.9 each

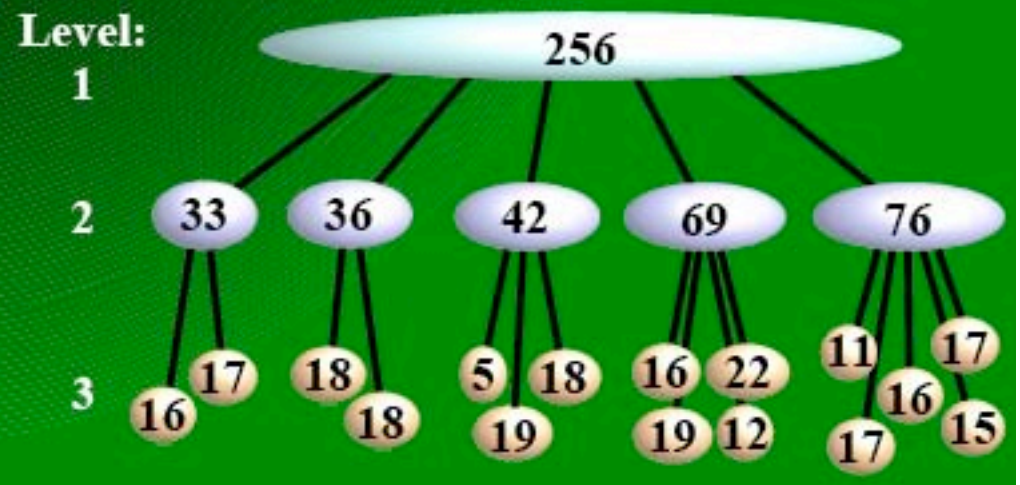
Multi-Resolution Test System: Hierarchical

- Test system is a heterogeneous 3-level hierarchy



Multi-Resolution Test System: Hierarchical

- Test system is a heterogeneous 3-level hierarchy
  - Level 1: 256 nodes with a random density of 0.1 between sub-communities
  - Level 2: 5 groups of sizes from 33 to 79 with an edge density of 0.3 each between sub-communities
  - Level 3: 16 groups of sizes from 5 to 22 with an interior edge density of 0.9 each



Multiresolution Test System

- (*i*a,b) → Level 2: 5 communities
- (*ii*a,b) → Level 3: 16 communities
- VI "peaks" → inter-communty edge density *or* maximum "complexity" at zero energy difference between states