Large-deviation properties of random graphs

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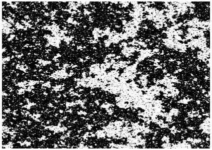
Computational Physics Group

Computer Science

Physics

helps →

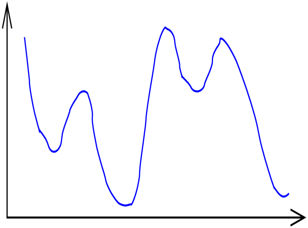
← helps



Computer simulations
new algorithms

Optimization algorithms
development/applications

[PPCC]



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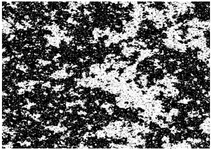

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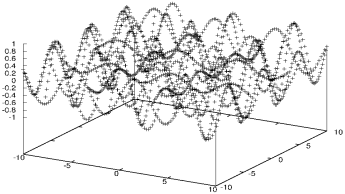


systems with 10^6 particles

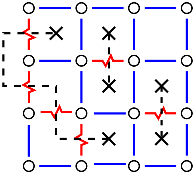
NEW:

[AKH, *Practical Guide to Computer Simulations*, World Scientific, 2009]

Disordered magnets

Spin glasses

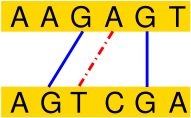
Random-field systems



Bioinformatics

RNA secondary structures

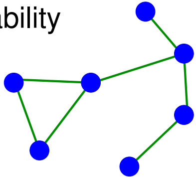
Sequence alignments



Phase transitions in optimization problems

Vertex cover

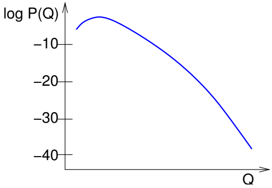
Satisfiability



Large-deviations properties

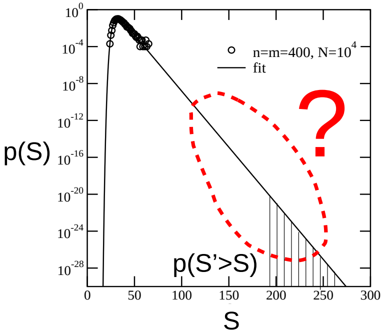
Disordered Systems

Random graphs



Large-deviation properties

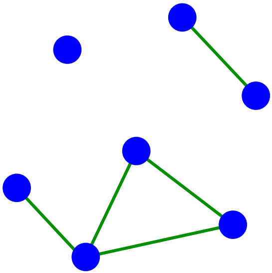
- Typical properties (probabilities $10^{-6}..1$): easy to get by simple sampling simulations
- Sometimes wanted: large deviation properties (of quenched-disorder ensembles)



- Examples:
  - Biological sequence (protein) alignment: small-probability (significant) scores [AKH, PRE 2001]
  - Distribution of the number of components of random graphs [A. Engel, R. Monasson, AKH, J. Stat. Phys. 2004]
  - Calculation of partition functions in statistical mechanics [AKH, Phys. Rev. Lett. 2005]

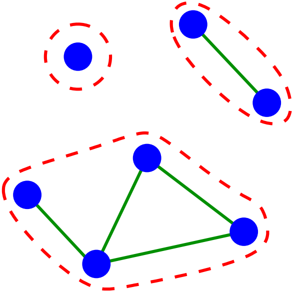
Graph ensembles

- Graph $G = (V, E)$



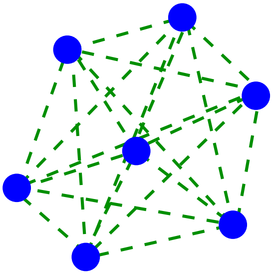
Graph ensembles

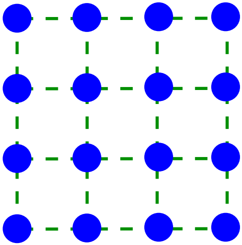
- Graph $G = (V, E)$
- connected components:
  transitive closure of “connectivity relation”



Graph ensembles

- Graph $G = (V, E)$
- connected components:
  transitive closure of "connectivity relation"
- Random graphs:
  here: N vertices, each edge tentative (ij) with prob. p.
  - Erdős-Rényi: $(ij) \in N^{(2)}$,
    $p = c/N \to$ finite connectivity c
  - two-dimensional percolation:
    $(ij) \in$ square lattice, $p =$ const



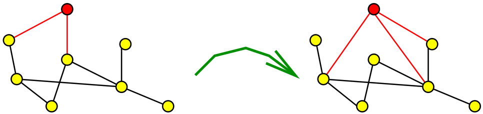


Physics Approach

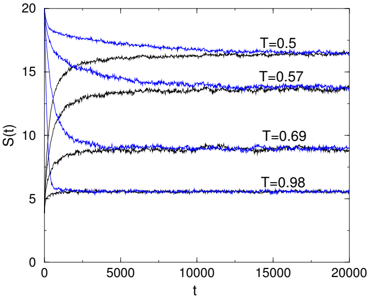
- Idea:

model	$\leftrightarrow$	physical system
quenched realisation	$\leftrightarrow$	degrees of freedom $\vec{x}$ (state)
quantity "score" S	$\leftrightarrow$	energy $E(\vec{x})$

  (ground state: often known)
  simulate at finite T
  Monte Carlo moves:
  change realisat. a bit



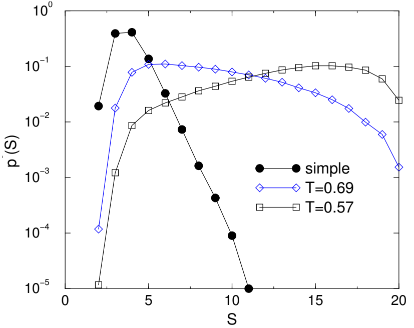
- Simulation at different T
  (using $(MC)^3$/PT)
  Example
  (sequence alignment)
  equilibration:
  start with ground state/
  with random state



- Wang-Landau approach

Distribution of Scores

- Raw result $\longrightarrow$
  (simple $\leftrightarrow T = \infty$)
  at low T:
  high scores prefered
- MC moves: $\vec{x} \to \vec{x}'$
  change on "element"
  probability $= f_a$



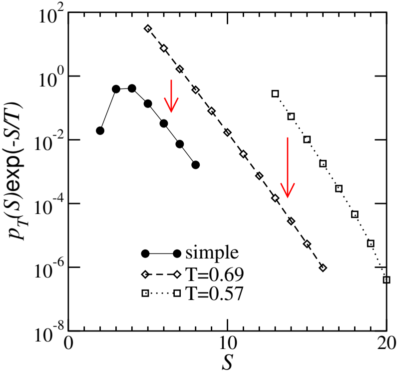
$$\Pr(\text{acceptance}) = \min\{1, \frac{\exp(S(\vec{x}')/T)}{\exp(S(\vec{x})/T)}\} = \min\{1, e^{\Delta S/T}\}$$

- $\Rightarrow$ equilibrium distribution $Q_T(\vec{x}) = P(\vec{x})e^{S(\vec{x})/T}/Z(T)$
  with $P(\vec{x}) = \prod_i f_{x_i}$, $Z(T) = \sum_{\vec{x}} P(\vec{x})e^{S(\vec{x})/T}$
  $\Rightarrow\ p_T(S) = \sum_{\vec{x},S(\vec{x})=S} Q_T(\vec{x}) = \frac{\exp(S/T)}{Z(T)} \sum_{\vec{x},S(\vec{x})=S} P(\vec{x})$
  $\Rightarrow\quad p(S) = p_T(S)Z(T)e^{-S/T}$ [AKH, PRE 2001]

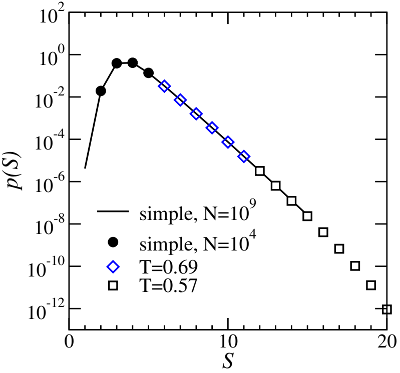
Match Distriutions

$\left[\ p(S) = p_T(S)Z(T)\exp(-S/T)\ \right]$

rescaling with $\exp(-S/T)$



$Z(T)$ by "matching"

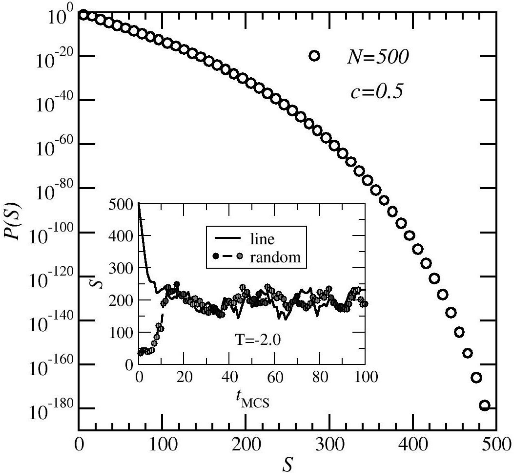


agrees with large statistics simple sampling

agrees with (for this example) known exact result

Results: Erdős-Rényi

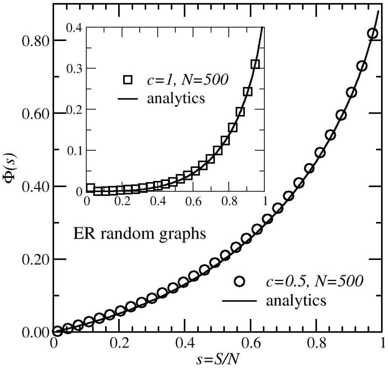
Size S of largest component (connectivity c)

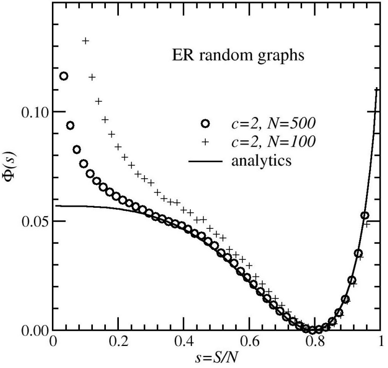


[AKH, Eur. Phys. J. B (2011)]

- Rate function $\Phi(s) \equiv -\frac{1}{N} \log P(s)$, $s = S/N$
- Comparison with exact asymptotic result

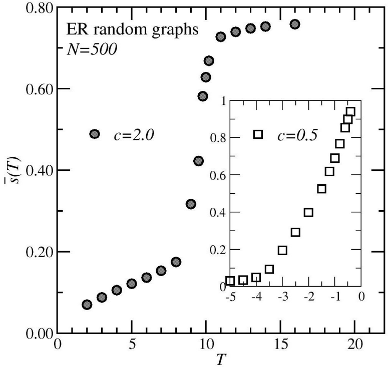
  [M. Biskup, L. Chayes, S.A. Smith, Rand. Struct. Alg. 2007]
- $\rightarrow$ evaluate algorithm $\rightarrow$ works very well
- $\rightarrow$ finite-size corrections visible

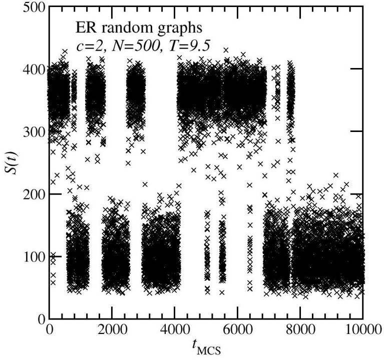




Phase transition

- Cluster size as function of (artificial) temperature
- 1st order transition in percolating phase

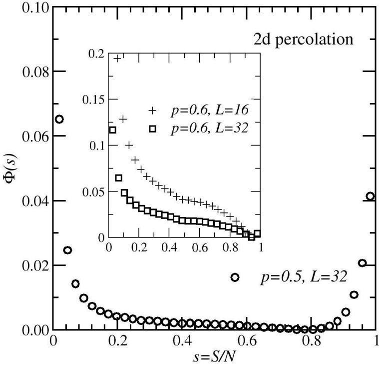


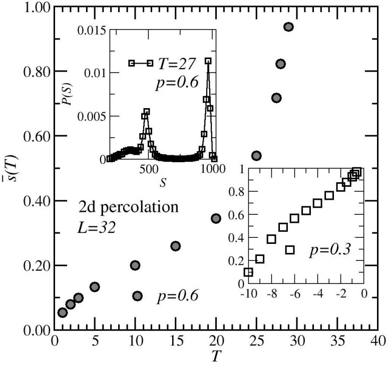


- → large system sizes not fully accessible

Two-dimensional percolation

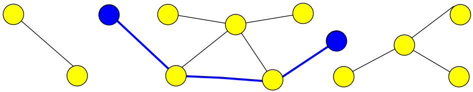
- $N = L \times L$, edge density p
- No exact result known (to me)
- Results comparable to Erdős-Rényi random graphs but stronger finite-size effects





Graph Diameter

- Diameter $d^\star$:= Longest of all shortest $i \to j$ paths



- Random graphs: ($c < 1$): Gumbel distribution

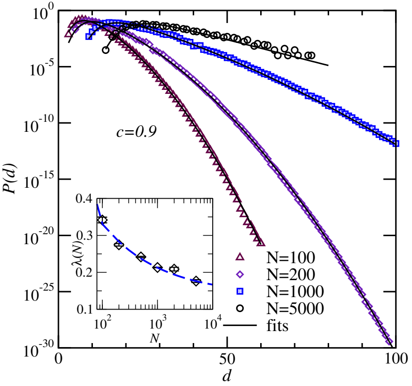
$$Pr_G(d^\star = d) = \lambda e^{-\lambda(d-d_0)} e^{-e^{-\lambda(d-d_0)}}$$

- Explanation:
  graph = forest
  d = $\max_{\text{trees } T} d(T)$
  $\to$ Gumbel distribution
- Fit to

$$P(d) = P_G(d) e^{-a(d-d_0)^2}$$

"gaussianized" Gumbel

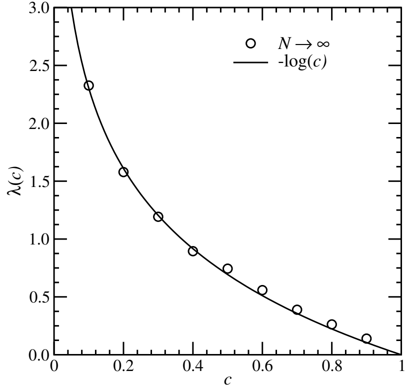
[AKH, M. Mézard, in preparation]



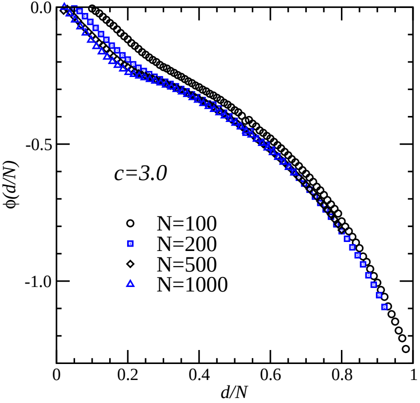
Close to $c = 1$, asymptotically

$$\lambda(c) = -\log c$$

[T. Luczak, Rand.Struct.Alg., 1998]



Percolating region:
more complex distributions



Summary

- Large-deviation properties
- Simulation approach:
  study system at artificial finite temperature
  (or, in principle, Wang-Landau algorithm $+$ modifications)
- Full distribution of size of largest component
- Erdős-Rényi random graphs: matches well analytics
  1st order transition in percolating phase
- 2d percolation: like ER model, stronger finite-size effects
- Distribution of number of components:
  agreement with statistical mechanics approach
- Distribution of diameter:
  $c < 1$: Gumbel distribution, matches theory
  $c > 1$: complex distribution, no theory