Large-deviation properties of largest component for random graphs

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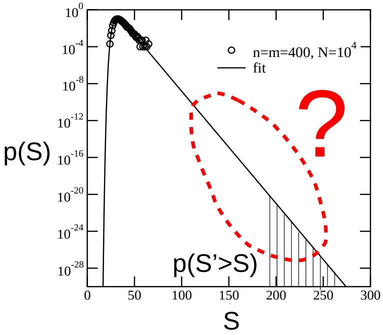
Outline

- Why large deviations?
- Graphs
- Algorithm
- Size of largest component of random graphs
- Two-dimensional percolation

DAAD summer academy
Modern Computational Science 2011:
Simulation of Extreme Events
15.-26. August 2011, University of Oldenburg
www.mcs.uni-oldenburg.de (2011 program soon)

Large-deviation properties

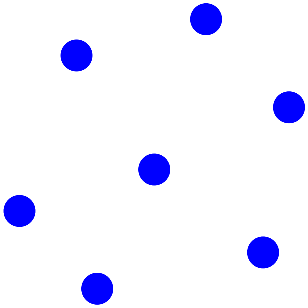
- Typical properties (probabilities $10^{-6}..1$): easy to get by simple sampling simulations
- Sometimes wanted: large deviation properties (of quenched-disorder ensembles)



- Examples:
  - Biological sequence (protein) alignment: small-probability (significant) scores [AKH, PRE 2001]
  - Distribution of ground-state energies of random magnets [M. Körner, H.G. Katzgraber, AKH, JSTAT 2006]
  - Calculation of partiction functions in statistical mechanics [AKH, PRL 2005]

Graphs

- Graph $G = (V, E)$
- V: set of vertices



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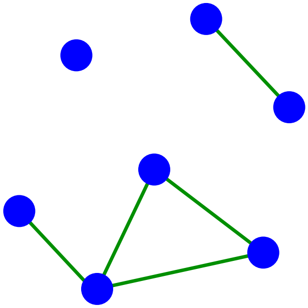
- $E \subset V^{(2)}$: set of edges
  for edge $(ij) \in E$:
  i, j are connected



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  transitive closure of
  “connectivity relation”
- no spacial structure, just
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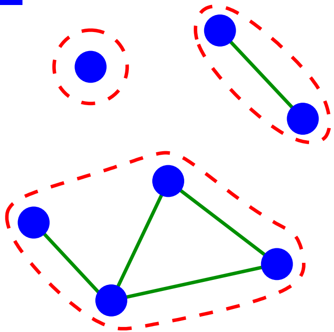

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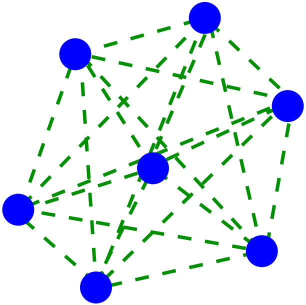


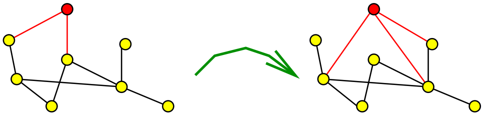
- Random graphs:
  here: N vertices, each tentative edge (ij) with prob. p.
  - Erdös-Rényi: $(ij) \in N^{(2)}$, $p = c/N \rightarrow$ finite connectivity c
  - two-dimensional percolation: $(ij) \in$ square lattice, $p = \text{const}$

Physics Approach

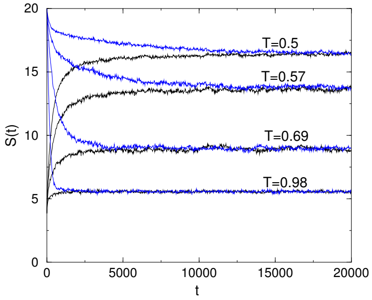
- Idea:

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

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

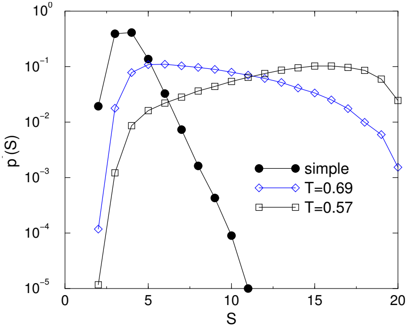


- Simulation at different T
  (using $(MC)^3$/PT)
  Example
  (sequence alignment)
  equilibration:
  start with ground state/
  with random state



Distribution of Scores

- Raw result $\longrightarrow$
  (simple $\leftrightarrow T = \infty$)
  at low T:
  high scores prefered
- MC moves: $c \to c'$
  change on “element”
  probability $= f_a$



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

- $\Rightarrow$ equilibrium distribution $Q_T(c) = P(c)e^{S(c)/T}/Z(T)$
  with $P(c) = \prod_i f_{x_i} \prod_j f_{y_j},\ Z(T) = \sum_c P(c)e^{S(c)/T}$

$$\Rightarrow\ p_T(S) = \sum_{c,S(c)=S} Q_T(c) = \frac{\exp(S/T)}{Z(T)} \sum_{c,S(c)=S} P(c)$$

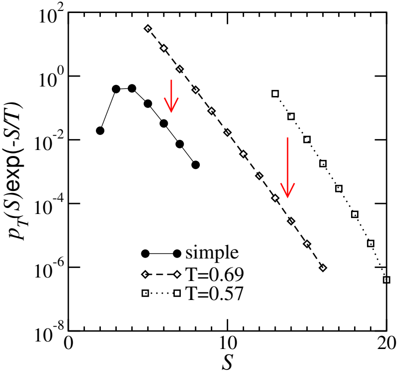
$$\Rightarrow \quad p(S) = p_T(S)Z(T)e^{-S/T}$$

[AKH, PRE 2001]

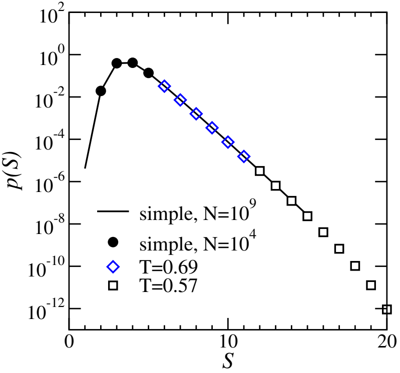
Match Distriutions

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

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



$Z(T)$ by “matching”

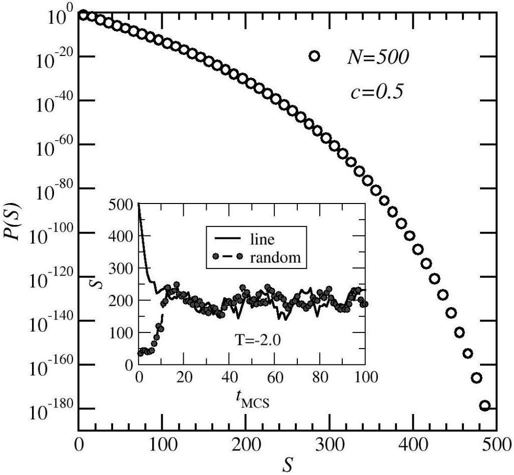


agrees with large statistics simple sampling

agrees with (for this example) known exact result

Results: Erdős-Rényi

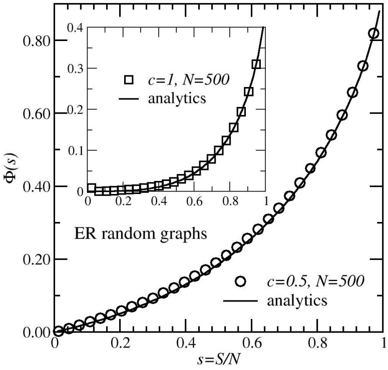
Size S of largest component (connectivity c)

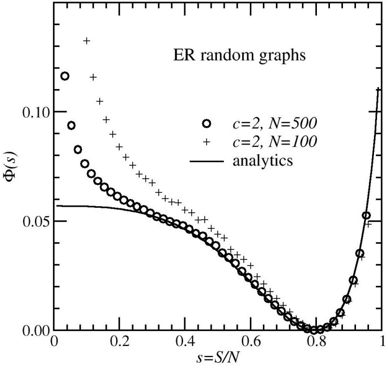


[AKH, arXiv:1011.2996 (2010)]

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

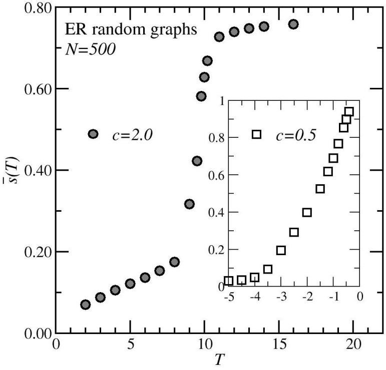
  [M. Biskup, L. Chayes, S.A. Smith, Rand. Struct. Alg. 2007]
- $\rightarrow$ evaluate algorithm $\rightarrow$ works very well
- $\rightarrow$ finite-size corrections visible

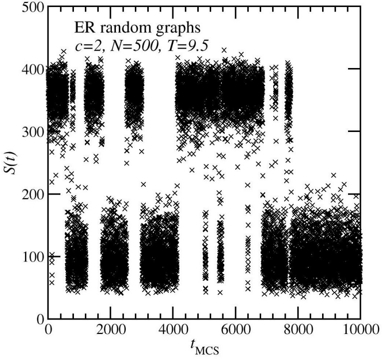




Phase transition

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

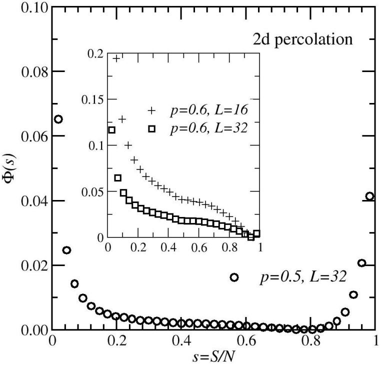


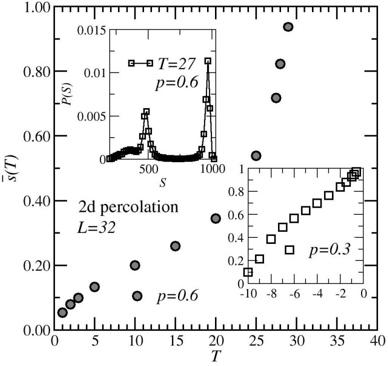


- → large system sizes not fully accessible

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





Summary

- Large-deviation properties
- Physics approach:
  study system at artificial finite temperature
  (or, in principle, Wang-Landau algorithm: here not effcient)
- Full distribution of size of largest component
- Erdős-Rényi random graphs: matches well analytics
  1st order transition in percolating phase
- Two dimensional percolation:
  comparable to ER model, stronger finite-site effects

[AKH, Practical Guide to Computer Simulations (World Scient., 2009)]