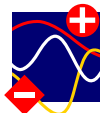


# Large-deviation properties of random graphs

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MAPCON 12, 15. May 2012



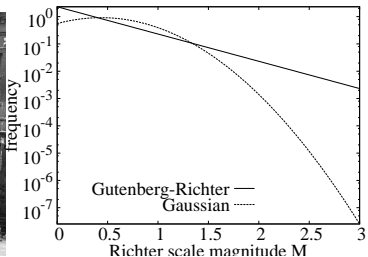
# Rare events

- Storms
- Stock-market crashes
- Floodings →
- Earth quakes ↓
- ...

Oldenburg August 2010



San Francisco 1906

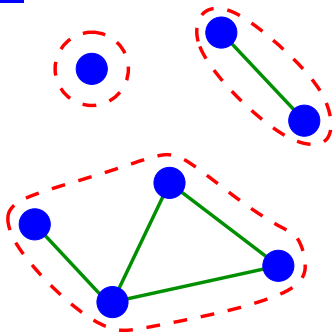


# Outline

- Algorithm
- Large-deviation graph properties  
(ER/2d lattice random graphs)
  - largest component
  - number of components
- Sampling of graphs

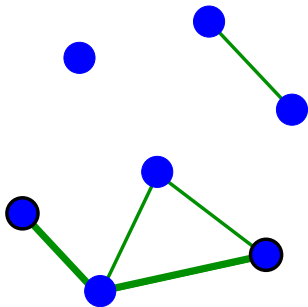
# Graphs

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



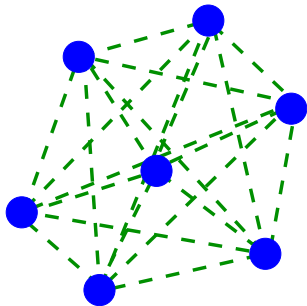
# Graphs

- Graph  $G = (V, E)$
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- **diameter**: longest among all pairwise shortest paths (within components)



# Graphs

- Graph  $G = (V, E)$
- **connected components**:  
transitive closure of  
“connectivity relation”
- **diameter**: longest among all  
pairwise shortest paths  
(within components)
- **Random graphs**:



$N$  vertices, each edge tentative  $(ij)$  with prob.  $p$ .

- Erdős-Rényi:  $(ij) \in N^{(2)}$ ,  $p = c/N \rightarrow$  finite connect.  $c$
- two-dim. **percolation**:  $(ij) \in$  square lattice,  $p = \text{const}$

$N$  vertices, given (sampled) degree sequence  $k_1, \dots, k_i$ ,  
e.g., scale-free  $P(k) \sim k^{-\gamma}$

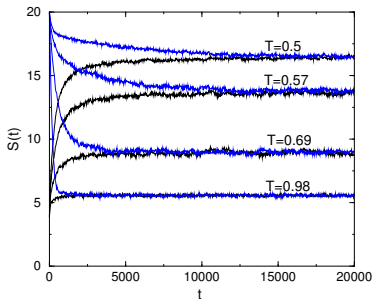
each graph with same probability (“configuration model”)

# 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 realisation a bit

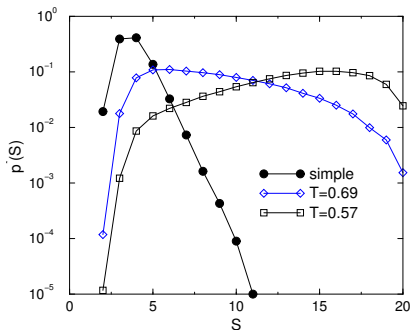


- Simulation at different  $T$   
(using (MC)<sup>3</sup>/PT)  
Example  
(sequence alignment)  
equilibration:  
start with ground state/  
with random state
- Wang-Landau approach



# Distribution of Scores

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



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

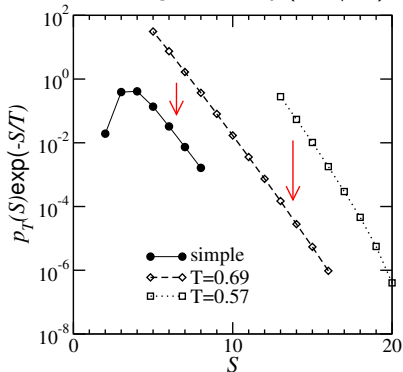
- $\Rightarrow$  equilibrium distribution  $Q_T(\vec{x}) = P(\vec{x})e^{S(\vec{x})/T}/Z(T)$   
with  $P(\vec{x}) = \prod_i f_{x_i}$ ,  $Z(T) = \sum_{\vec{x}} P(\vec{x})e^{S(\vec{x})/T}$
- $\Rightarrow p_T(S) = \sum_{\vec{x}, S(\vec{x})=S} Q_T(\vec{x}) = \frac{\exp(S/T)}{Z(T)} \sum_{\vec{x}, S(\vec{x})=S}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



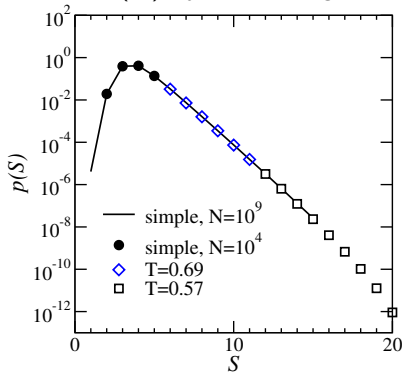
# Match Distributions

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

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



$Z(T)$  by "matching"

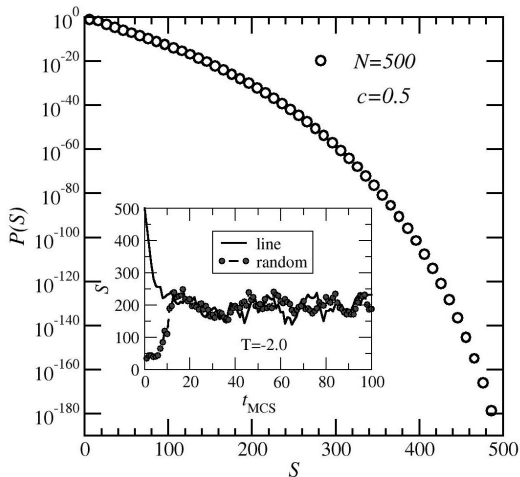


agrees with large statistics simple sampling

agrees with (for this example) known exact result

# Results: Erdős-Rényi

Size  $S$  of largest component (connectivity  $c$ )



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

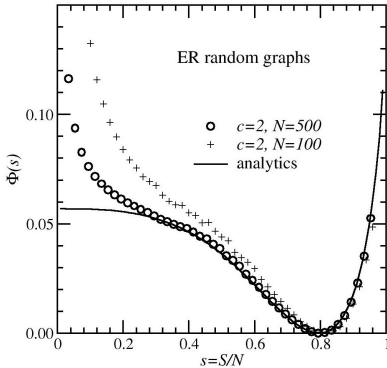
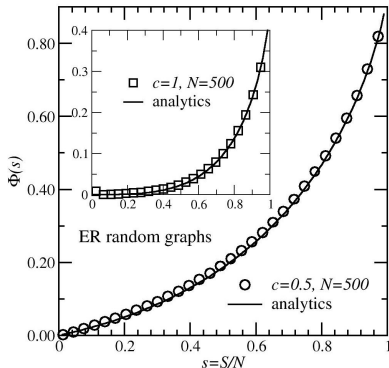
■ Rate function  $\Phi(s) \equiv -\frac{1}{N} \log P(s)$ ,  $s = S/N$

■ Comparison with exact asymptotic result

[M. Biskup, L. Chayes, S.A. Smith, Rand. Struct. Alg. 2007]

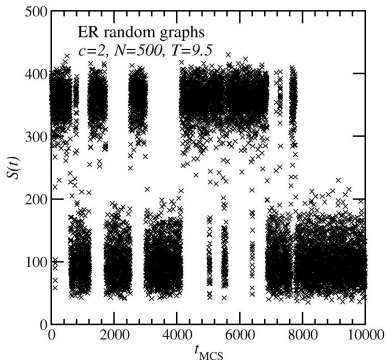
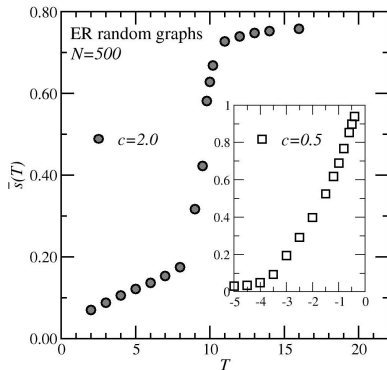
■  $\rightarrow$  evaluate algorithm  $\rightarrow$  works very well

■  $\rightarrow$  finite-size corrections visible



# Phase transition

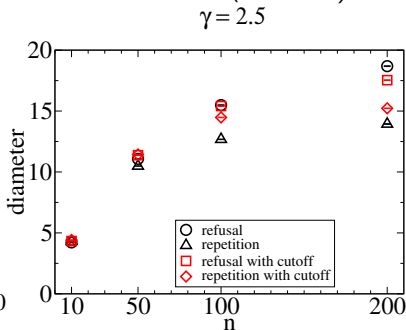
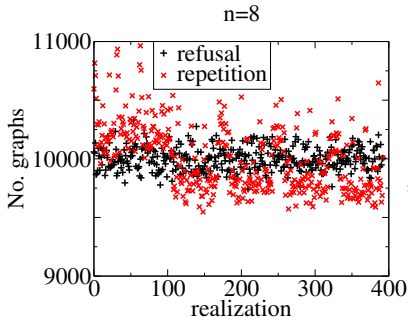
- Cluster size as function of (artificial) temperature
- 1st order transition in percolating phase



- large system sizes not fully accessible (→ use Wang-Landau algorithm here)

# Bias in Configuration model

- Configuration model:  $k$  “stubs” for each node of degree  $k$ . Randomly draw pairs of stubs. If multiple/self edge:
  - refusal: start graph from scratch
  - repetition: redraw pair
- Repetition is biased: relevant for measurements ( $N \rightarrow \infty$ )?

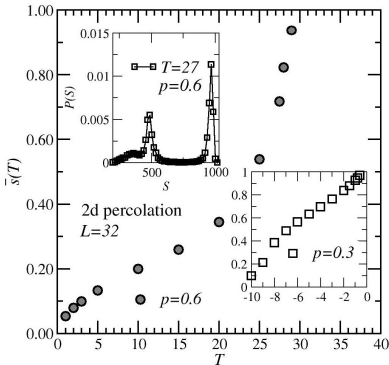
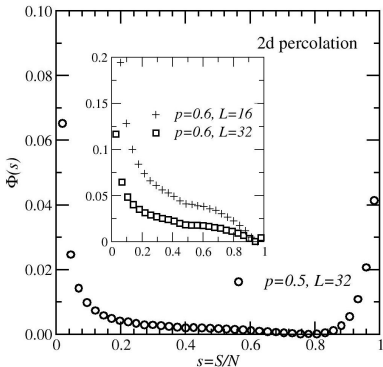


[H. Klein-Hennig, AKH, Phys. Rev. E 2012]

- → Markov chains/ hidden variables/ throw-away edges/ ...

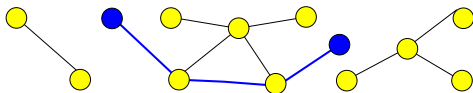
# Two-dimensional percolation

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



# Graph Diameter

- Diameter  $d^* :=$   
Longest of all  
shortest  $i \rightarrow j$  paths



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

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

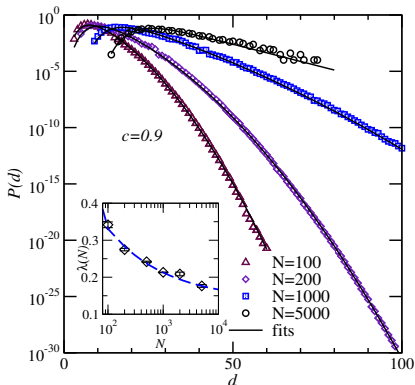
- (sloppy) explanation:  
graph = forest  
 $d = \max_{\text{trees}} \tau d(T)$   
→ Gumbel distribution

- Fit to

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

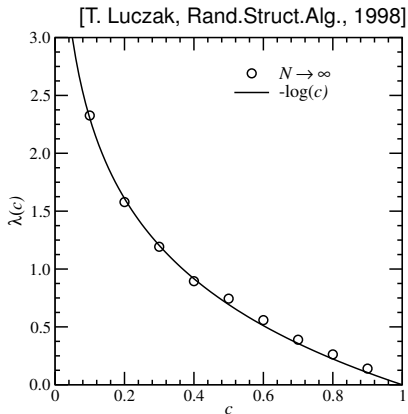
“gaussianized” Gumbel

[AKH, M. Mézard, in preparation]

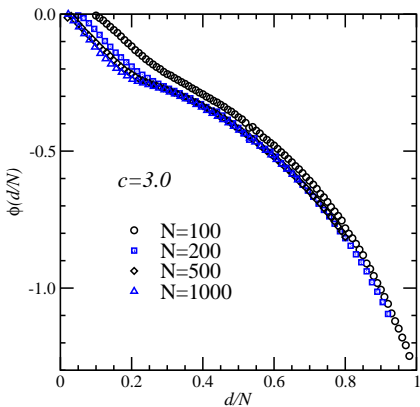


Close to  $c = 1$ , asymptotically

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



Percolating region:  
more complex distributions





# Summary

- Large-deviation properties
- Physics 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  
(also: number of components, 2d percolation, diameter)
- Simple sampling of configuration model is biased

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Summer school: Efficient Algorithms in Computational Physics  
Bad Honnef (Germany), 10-14. September 2012