Phase transitions in combinatorial optimization problems
Course at Helsinki Technical University, Finland, autumn 2007
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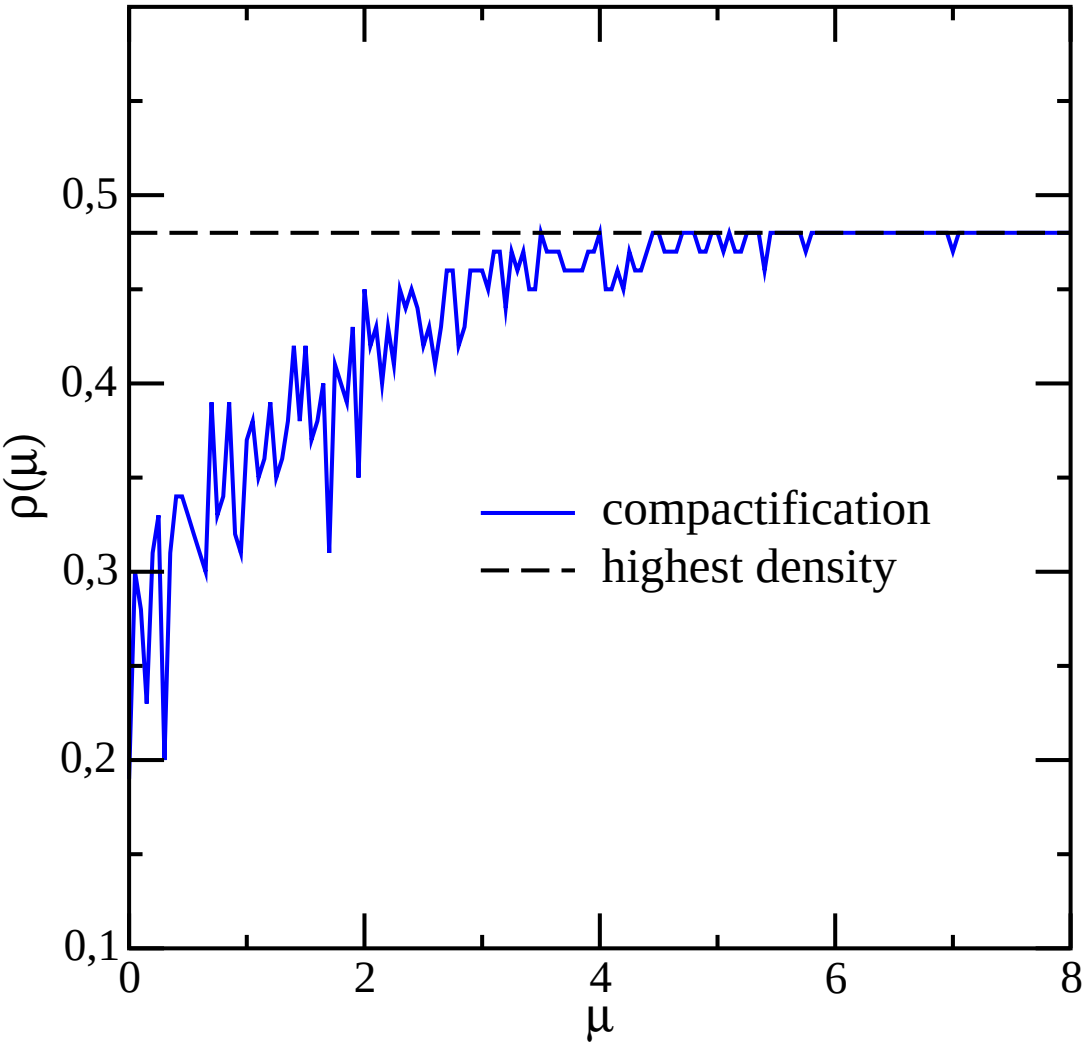
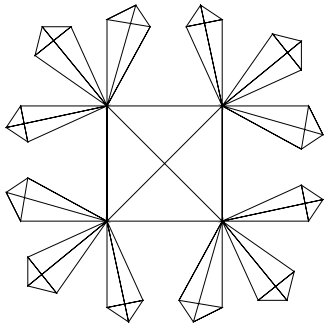
Lecture 6, 4. October 2007

One MC sweep: exactly N tried transitions, each time randomly selecting a vertex.
Example: compactification of a hard-core gas ($N = 100$ with connectivity $c = 4.0$): start with $\mu = 0$, then μ is gradually increased by $\delta\mu = 0.05$ up to $\mu_f = 8$. (for each μ, 10 MC sweeps) density ρ/N measured.



One run, algorithm finds true VC, MC works fine here.

Other ensemble: random graphs made of randomly joined tetrahedrons (cliques of size 4):



Algorithm gets stuck in meta-stable configurations (lower density)
Reason: configuration space has a very complicated and rugged structure.
(see M. Weigt and A.K. Hartmann, "Glassy behavior induced by geometrical frustration in a hard-core lattice gas model", Europhys. Lett. **62**, 533 (2003))

RS Analytics → obtaining local densities ρ_i: two solutions obtained: "liquid" (L, $\rho_i = \overline{\rho}$) and "crystal" (C, $\rho_i = \rho_1$ or $\rho_i = \rho_2$, $\rho_1 < \rho_2$, all neighbors j of i with $\rho_i = \rho_2$ have $\rho_j = \rho_1$)

- $0 \leq \mu < \mu_s$: only L solution exists
- $\mu_s < \mu < \mu_c$: L,C exists, L has higher weight
- $\mu_c < \mu < \mu_d$: L,C exists, C has higher weight (L is "metastable" → super-cooled liquid)
- $\mu_d < \mu < \mu_{rsb}$: appearance of exponentially many glassy solutions (many different ρ_i), but lower weight than L
- $\mu_{rsb} < \mu < \infty$: some glassy solutions have higher weight than L (1-RSB) (but lower than C → only dynamics affected)

For glassy systems better algorithm, see next section.

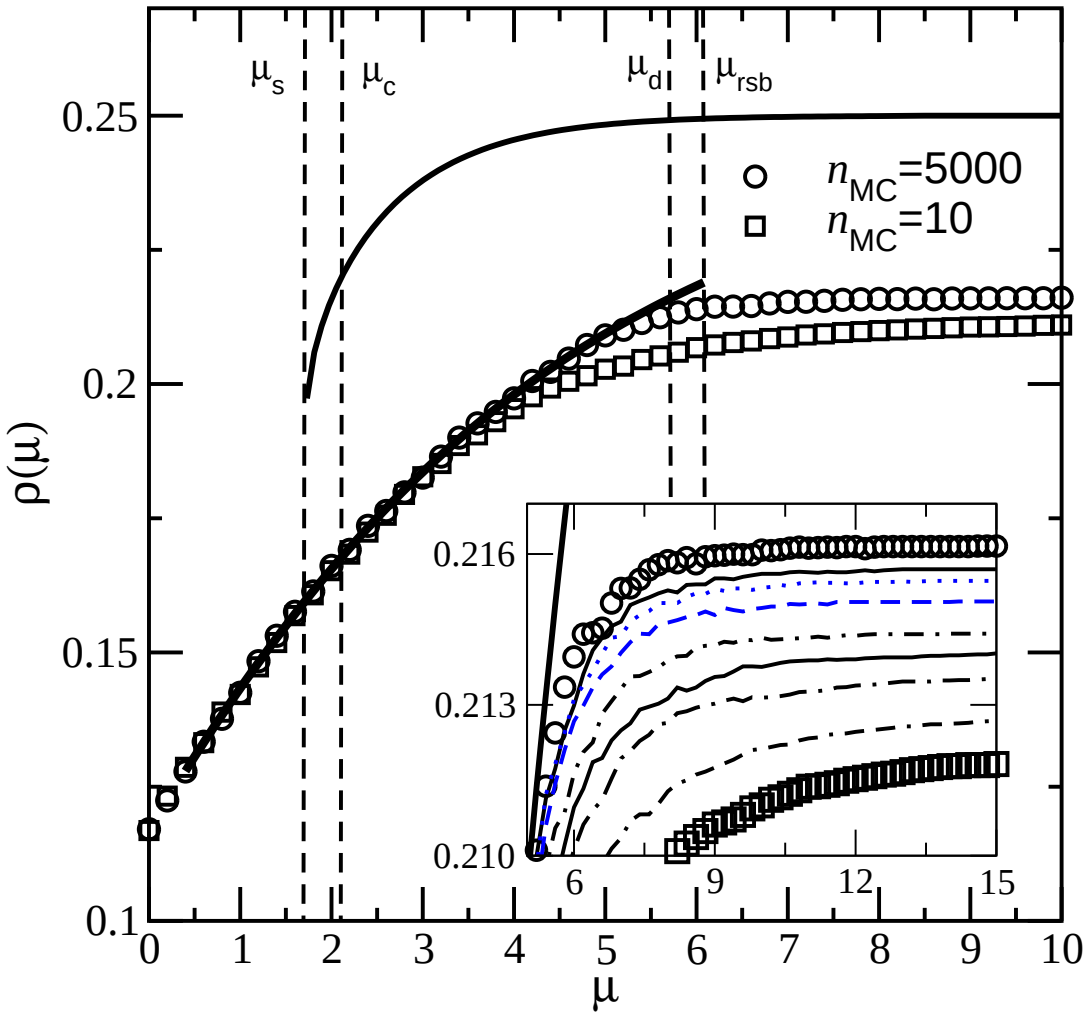


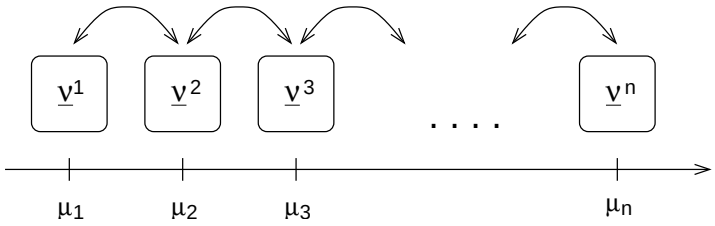
Figure 1: Density ρ as a function of the chemical potential μ, for $p = 4$, $K = 3$. The full lines give analytical results for the liquid and the crystalline phases. The spinodal and the crystallization points, as well as the dynamic and static glass transition are marked by vertical lines (from left to right). Results are compared with numerical compaction curves for random generalized Bethe lattices of size $N = 999$, averaged over 100 graphs. Here $\delta\mu = 0.2$ was used. Inset: Compaction rate dependence for high values of μ for $n_{\rm MC}$ ranging from 5000 (top) to 10.

3.6 Parallel tempering

(also called MC^3 = Metropolis-coupled Monte Carlo Markov Chain)

- C. Geyer "Monte Carlo Maximum Likelihood for Depend Data", Proceedings of the 23rd Symposium on the Interface, 156-163 (1991)
- K. Hukushima and K. Nemoto, J. Phys. Soc. Jpn. **65**, 1604 (1996)

basic idea: simulate several copies of same system, but different configurations, at $\mu_1 < \mu_2 < \ldots < \mu_n$



1. each config: treated by MC as above (M, E moves)
2. additional: swap (S) transition: exchange configs at μ_k, μ_{k+1} ($k \in [1, n-1]$)
   → Allows configs to visit different μ values → overcoming energy barriers

Important: detailed balance must still hold →

S move:

1. choose $k \in \{1, 2, \ldots, n-1\}$ randomly
2. Let $\underline{\xi}, \underline{\zeta}$ be configs at values μ_k,μ_{k+1}.
   Joint probability:

$$P_{k,k+1}(\underline{\xi}, \underline{\zeta}) = \frac{1}{\tilde{\Xi}_{k,k+1}} \chi(\underline{\xi}) \exp\left(\mu_k \sum_i \xi_i\right) \chi(\underline{\zeta}) \exp\left(\mu_{k+1} \sum_i \zeta_i\right), \qquad (1)$$

   ($\tilde{\Xi}_{k,k+1}$: normalization)

$$\text{Let} \quad \Delta_{k,k+1}(\underline{\xi}, \underline{\zeta}) \equiv (\mu_k - \mu_{k+1}) \left(\sum_i \xi_i - \sum_i \zeta_i\right) \qquad (2)$$

   ⇒ perform swap with prob.

$$W_{k,k+1}([\underline{\xi}, \underline{\zeta}] \rightarrow [\underline{\zeta}, \underline{\xi}]) = \exp(-\max[\Delta_{k,k+1}(\underline{\xi}, \underline{\zeta}), 0]) \,. \qquad (3)$$

Proof of detailed balance: excercise!

In practice: choose

- range of μ values
- number n of μs
- values of μ_i
- ration between S and E,N moves

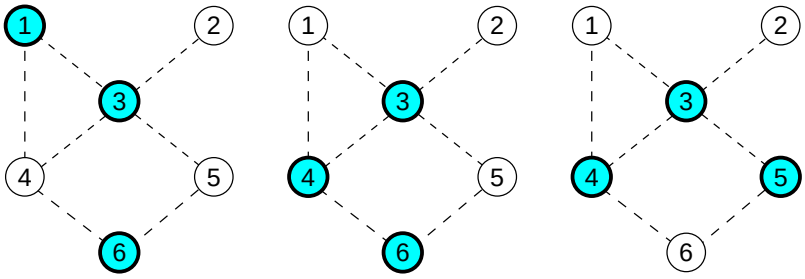
Rule of thump: acceptance = 0.5 for S move.
$\rightarrow$ $N = 1000$ Erdős Réyni graphs possible

3.7 Backbone

Min. VCs may be not unique $\rightarrow$ several (min.) covers $V_{\rm vc}^{(1)}$, ..., $V_{\rm vc}^{(K)}$.

Backbone vertex: either $(\forall k = 1, \ldots, K : i \in V_{\rm vc}^{(k)})$ or $(\forall k = 1, \ldots, K : i \notin V_{\rm vc}^{(k)})$.

Example: Minimum vertex cover
Graph with three minimum VCs ($X_{\rm c} = 3$)



Backbone: Vertices 2 (always uncovered) and 3 (always covered)

Vertex 3 must be a member of all minimum VCs: If no covered all is $4 > 3 = X_{\rm c}$ neighbors must be covered. □

Obtaining backbone B:

Simple: Enumerate all solutions using B&B algorithm and check which vertices appear with different assignments. Problem: Usually there are exponentially many solutions.

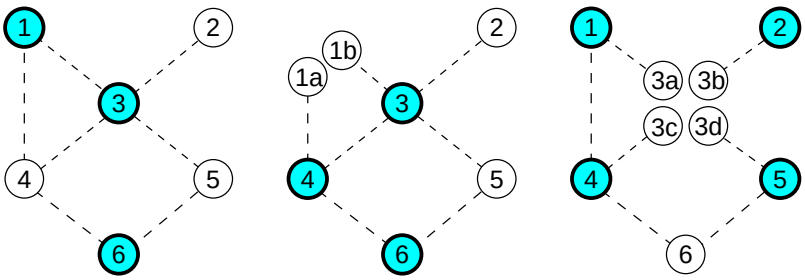
Better: since $B = B^{ac} \cup B^{auc}$

algorithm backbone(G)
begin
  calculate one min cover $V_{\rm vc}^1$ of G

  comment calculate always-covered backbone:
  for all $i \in V_{\rm vc}^1$ **do**
  if degree $d_i = 1$ **then**
    i is not in the backbone
  else
  begin
    create new graph G':
      remove i
      for each dangling end of edges **do**
        add one vertex at the dangling end
    calculate min cover $V'_{\rm vc}$ of G'
    if $|V'_{\rm vc}| > |V_{\rm vc}^1|$ **then**
      i is in backbone
    else
      i is not in backbone
  end

  comment Calculate always-uncovered backbone vertices:
  for all vertices i which have only ac backbone neighbors:
    i is in backbone (uncovered)
  comment also vertices with degree 0 are backbone (uncovered)
end

Example: Backbone algorithm



Left: one minimum cover $V_{\rm vc}^1$
Vertices 1, 3 and 6: candidates for the ac backbone.

Middle: The modified graph G' for vertex 1
Size of the min. VC = size of $V_{\rm vc}^1$

→ Vertex 1 is not backbone

Right: modified graph for vertex 3.
Min. VC than $|V_{\rm vc}^1|$
→ vertex 3 member of B^{ac}.

Finally $B^{ac} = \{3\}$
Vertex 2: only one with only neighbors in B^{ac}
→ $B^{auc} = \{2\}$. □

Result from simulation <u>at</u> $x_{\rm c}(c)$
Note: for $x > x_c$: <u>no</u> backbone

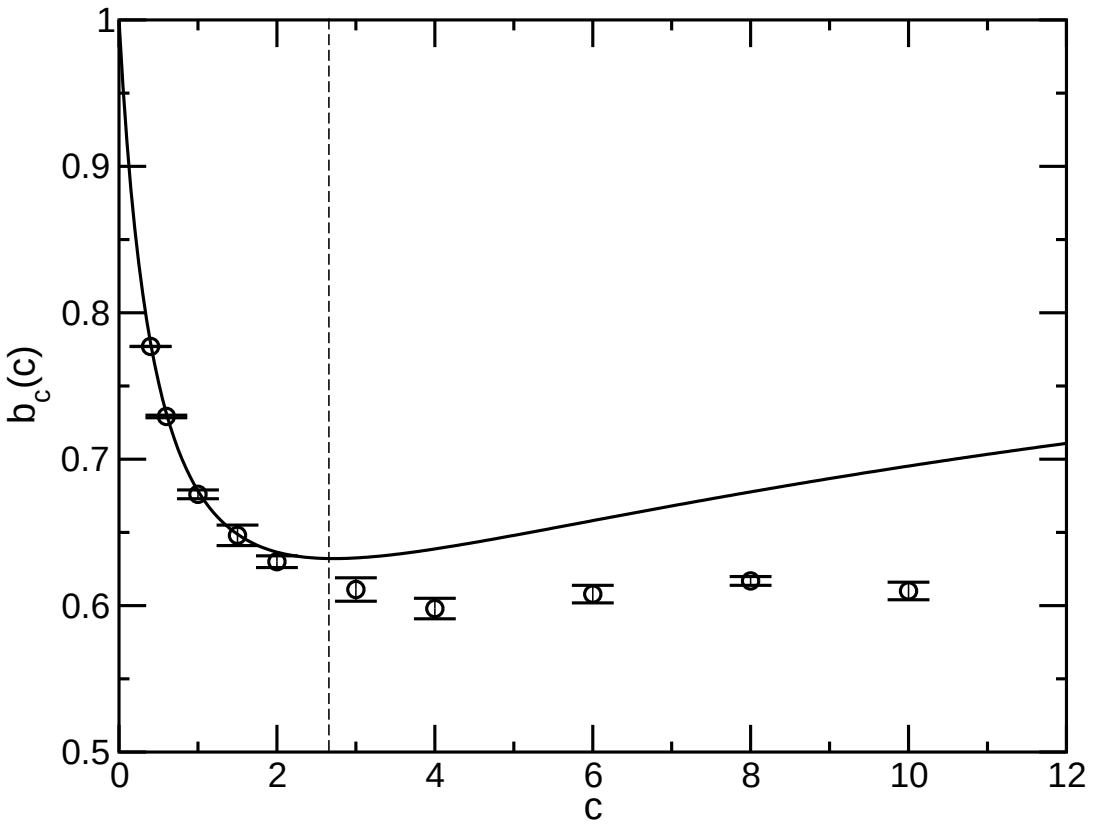


Figure 2: The total backbone size of minimum vertex covers as a function of c. The solid line shows the analytical result. Numerical data are represented by the error bars. They were obtained from finite-size scaling fits similar to the calculation for $x_{\rm c}(c)$. The vertical line is at $c = e \approx 2.718$ where the analytical results cease to be exact.