Phase transitions in combinatorial optimization problems Course at Helsinki Technical University, Finland, autumn 2007 by Alexander K. Hartmann (University of Oldenburg) Lecture 4, 27. September 2007

Remarks: Outline of Talk shoould be slide-wise, i.e. few keywords per slide.

(show sample talk of myself)

Missing appointments

3.3 Numerical Results

Ensemble $\mathcal{G}(N, c/N)$ of random graphs: N vertices, each poss. N(N-1)/2 edge is present with prob. c/N. $\rightarrow c =$ average degree Here: c = 2.0.



Figure 1: Probability $P_{cov}(x)$ that a VC exists for a random graph (c = 2) as a function of the fraction x of <u>covered</u> vertices.

Three different system sizes N = 25, 50, 100 (averaged over $10^3 - 10^4$ random graphs).

Left: average energy density e(x).

Inset: result for the energy in the region $0.3 \le x \le 0.5$.



Figure 2: Time complexity of the vertex-cover algorithm = median number of nodes visited in the configuration. N = 20, 25, 30, 35, 40,c = 2.0. Right part (x > 0.4): Running times grows linearly. Inset: logarithmic scale (also N = 45, 50) \rightarrow time complexity grows exponentially with N.

Finit-Size Scaling

(1)

Determine $x_{\rm c}(N)$ for different graph sizes N fit to the data a function

$$x_{\rm c}(N) = x_{\rm c} + aN^{-b}$$

(frequently found behavior in physical systems)



Matches well:



Figure 3: Finite-size scaling behavior of the critical cover size. The location of the transition point $x_c(N)$ as a function of graph size N for different average degree c. Inset: scaling of the correlation volume as a function of x for different sizes. Error bars are, at most, of the order of the symbol size.

b does not depend much on the connectivity c: b(c = 2) = 0.91(9), b(3) = 0.88(4), b(4) = 0.82(4), b(6) = 0.92(11)



Figure 4: Phase diagram. Circles: numerical simulations. Line: analytical result. Bounds: dashed/dashed-dotted lines. Vertical line at $c = e \approx 2.718$.

Analytical Result:

$$x_{\rm c}(c) = 1 - \frac{2W(c) + W(c)^2}{2c}, \qquad (2)$$

W(c): Lambert-W function: $W(c) \exp(W(c)) = c$. Result exact until $c = e \approx 2.718$: Assumption of <u>Replica symmetry</u> (RS) (\leftrightarrow simple organisation of phase space) is true.

c>e: Replica symmetry breaking (RSB) (\leftrightarrow complex phase space) \rightarrow cannot be calculated exactly here.



Note: percolation at $c_{\rm crit} = 1.0 < e$!

3.4 Leaf-Removal algorithm

Speed up for finding minimum-size VCs (optimization problem 2)

Basic idea: only full VCs wanted

- $\rightarrow \underline{\text{all}} \text{ edges must be covered}$
- $\rightarrow \underline{\text{all}} \text{ edges } \{i, l\} \text{ to } \underline{\text{leaves }} l \text{ (degree 1) must be covered}$
- \rightarrow either i or l must be covered
- \rightarrow no harm in covering i, i.e. neighbours of leaves.
- \rightarrow all edges incident to *i* are covered
- \rightarrow maybe more leaves generated

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algorithm leaf-removal (G = (V, E))

begin

Initialize V' = \emptyset

while there are leaves i (i. e.vertices with degree d_i = 1) do

begin

Let j be the neighbor of a leaf i

cover j, i. e., V' = V' \cup \{j\}

Remove all edges adjacent to j from E

Remove i and j from V

end

return (V')

end
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Running time: $\mathcal{O}(M) (= O(N)$ for random graphs with fixed c)

Remaining graph: called <u>core</u>

Each component of core: treated with brand-and-bound algorithm.

Example: Leaf removal



Figure 5: Example of the leaf-removal algorithm. Upper left: initial graph, vertices 1 and 2 are leaves. Upper right: graph after the first iteration, vertex 5 has been covered (shown in bold) and the incident edges removed (shown with dashed line style). Bottom: graph after second and third iteration.

Previous sample graph Two leaves, vertices 1 and 2

Iteration 1: say vertex 5 (neighbor of 2) is <u>covered</u>. (edges $\{2, 5\}$ and $\{5, 8\}$ are covered and removed)

It. 2: v. 3 <u>covered</u> (neighbor of 1) (\rightarrow edges {1,3} and {3,6}) \rightarrow new leaf (vertex 6)

It. 3: v. 7 <u>covered</u> (neighbor of 6) \rightarrow just one egde left (i.e. two leaves 4,8) It. 4: v. 8 covered \rightarrow min. VC found!

Note: for random graphs, connectivities c < e: core is not extensive \rightarrow core = collections of components of $\mathcal{O}(\log N)$ (Bauer and Golinelli, Europ. Phys. J. B 24, 339 (2001))

 \rightarrow per component: running time of brand-and-bound algorithm exponential in $\log N,$ i.e. polyonmial in N

 \rightarrow min VC can be found typically in $\mathcal{O}(N^k)$ for c < e.

3.5 Monte Carlo (MC) simulations

General simulation approach used in (statistical) physics. See books:

- M. E. J. Newman und G. T. Barkema, <u>Monte Carlo Methods in Statistical Physics</u> (Clarendon Press, Oxford, 1999).
- D. P. Landau and K. Binder, <u>A Guide to Monte Carlo Simulations in Statistical Physics</u>, (Cambridge University Press, Cambridge 2000).

Works very well for VC on random graphs, even for large c.

Basic idea: interpret VCs as configuration of physical system, a <u>hard-core lattice gas</u>, MC introduces a <u>dynamics</u> into the system. Idea: dynamic is guided to lead into minimum VCs.

3.5.1 The hard-core lattice gas

Arbitrary covers V_{vc} on graph G = (V, E) including those larger than the minimum VC:

 \rightarrow at least at one end-point of any edge there is a covering mark

Define <u>uncovered</u> vertices as occupied by particles.

 \rightarrow <u>not</u> allowed: particles at both endpoints of an edge particles have <u>chemical radius</u> of one = a hard-core repulsion

