Phase transitions in combinatorial optimization problems Course at Helsinki Technical University, Finland, autumn 2007 by Alexander K. Hartmann (University of Oldenburg) Lecture 1, 11. September 2007

1 Introduction

1.1 Technicalities

Survey: 5 CS students, 5 Physics students

Rules for <u>credits</u>: Presentation (about 30-60 minutes using beamer) + written Summary (5-10 pages, best latex) "Workshop" on Friday 12 October Test presentations on request (highly recommended, otherwise risk of no credit !!) alternative: programming project (only 1 or 2, on request) next lecture: Wed 12, 12-14 no lectures: 2nd week

tutorials: Fri 10-12 (from third week on)

- discussion/question hours
- special subjects on request (introduction to computational complexity, statistical physics, replica calculation, ...)
- presentations (12 October)

1.2 Examples

What is optimization: In school: find maximum/minimum of function.

In Reality: many variables, often discrete: $\underline{\sigma} = (\sigma_1, \ldots, \sigma_n) \in X^n$, (e.g. $X = \{0, 1\}, X = \mathbb{Z}$), $H(\underline{\sigma}) = \text{cost function}$. minimization problem

Find $\underline{\sigma} \in X^n$, which minimizes H!

 $\max H = -\min(-H)$ constraints: decrease number of feasible solutions.

In economics: save resources/money/time etc.

Aim: Measure running time as a function of "input size".

Reminder: **Definition:** O notation Let T, g be functions from $\mathbb{N} \to \mathbb{R}$ We write $T(n) \in O(g(n)) :\Leftrightarrow \exists c > 0$ with $T(n) \leq cg(n) \forall$. We say: T(n) is of order at most g(n).

Worst-case running time: $T_{wc}(n) = \max_{\text{all instances } I \text{ withsize } n} T(I)$ (traditional CS) <u>Typical running time</u>: Esemble of instances I of size n: average $T^*(n) := \langle T(I) \rangle_n$ or (better) median.

Example: Traveling Salesman Problem (TSP)

n cities distributed in a plane.

Find the shortest round-tour through all cities, each city only once.

$$X = \{1, 2, \dots, n\}$$
(1)

$$H(\underline{\sigma}) = \sum_{i=1}^{n} d(\sigma_i, \sigma_{i+1})$$
(2)

 $d(\sigma_{\alpha}, \sigma_{\beta})$: distance between cities; $\sigma_{n+1} \equiv \sigma_1$.





Algorithms: worst-case running time increases exponentially with n

In physics: ground state of magnetic systems, protein folding, data analysis, flux lines in superconductors

Example: Ising Spin Glasses

Ising spin $\sigma_i = \pm 1$, simple lattice, nearest neighbor interactions (ferromagnetic/antiferromagnetic).

$$X = \{-1, 1\}$$
(3)

$$H(\underline{\sigma}) = -\sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j \tag{4}$$

bonds $J_{ij} = \pm 1$. For each system: bonds fixed (quenched disorder) \rightarrow Average over many samples.

Ground state=minimum of energy.



Figure 2: Two-dimensional spin glass. Solid lines = ferromagnetic interactions, jagged lines = antiferromagnetic interactions, small arrows = spins in ground state, crosses = unsatisfied interactions.

In 2d: fast algorithms, in 3d only slow algorithms.

1.3 Why studying combinatorial optimizations using physics

Many practical optimization problems, also in physics Optimum cost function \leftrightarrow minimum energy \leftrightarrow ground state (T = 0)What makes a problem hard, related to glassiness? Phase transitions \leftrightarrow easy/hard changes Transformations to physical systems \rightarrow methods from stat. mech. Fast algorithms wanted: e.g. <u>simulated annealing</u> (old), <u>survey propagation</u> (new) Analysis of algorithms.

Example: Phase transitions in the TSP Plane area $A = L_x \times L_y$ Euclidean distances: $d(i, j) = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$ For each instance:

Is the shortest round trip through all cities shorter than a given length l?

Solve exactly using branch-and-bound algorithm (see later)

Result: probability p of tour length < l as function of rescaled length $\Phi = l/\sqrt{nA}$ 1. l scales with lengthscale of system, for constant n, i.e. \sqrt{A} . 2. l scales like A for constant density n/A. (Argument seems not work for d > 2, according analytic arguments.)



→ Drastical change at $\Phi = \Phi^* \approx 0.78$ phase transition rescaling: p as fct of $r = (\Phi - \Phi^*)n^{2/3}$ → data collaps (one curve)!

Running time: (mesured in terms of assigning city positions \rightarrow machine independent)



Instances close to phase transition: hardest to solve! Problem easy to solve for small/large values of l (i.e. Φ):

- Small l, even the two closest cities have a distance $> l \rightarrow$ algorithm terminates
- Large l, even random permutation has total distance < l.

1.4 Bibliography

(Handout: B. Hayes, can't get no satisfaction)

- A.V. Aho, J.E. Hopcroft, J.D. Ullman: The design and analysis of computer algorithms, Addison-Wesley 1974 (ebay!)
- T.H. Cormen, S. Clifford, C. E. Leiserson, R. L. Rivest: Introduction to Algorithms, MIT Press 2001
- M.R. Garey und D. S. Johnson: Computers and intractability, Freeman, New York, 1979
- A.K. Hartmann und M. Weigt: Phase Transitions in optimization problems, Wiley-VCH, Berlin 2005
- B. Hayes: On the Threshold, American Scientist **91**, 12 (2003)
- K.H. Fischer and J.A. Hertz: Spin Glasses, Cambridge University Press, 1991
- S. Mertens: Computational Complexity for Physicists, Computing in Science & Engineering 4(3), 31 (2002)
- C.H. Papadimitriou und K. Steiglitz: Combinatorial Optimization, Prentice-Hall 1982

1.5 Subjects of Seminar

(details: see http://www.tcs.hut.fi/Studies/T-79.7003/)

- Phase transition in the Number-Partitioning Problem
- Modern Walk-SAT algorithms
- Calculation of phase boundary for vertex-cover problem (analytical) [presented by: Joni Parjinen]
- Calculation of typical running time of a branch-and-bound algorithm for the vertex-cover problem (analytical)
- Calculation of typical running times of WalkSAT algorithms (analytical)
- Generating hard but solvable SAT formulas (bit analytical)
- Phase transitions in generalized SAT problems
- Phase transition in minimizing spin-glass energies
- Vertex-cover on other graph ensmbles (bit analytical)
- Phase transition in ground states of random-field systems and running time of maximum-flow algorithms

- Combinatorial auctions [presented by: Olli Ahonen]
- Uniform sampling of local minima in Ising spin glasses [presented by: Petri Savola]