Some practical experiences of hard graph problems

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BT Research at Martlesham, Suffolk

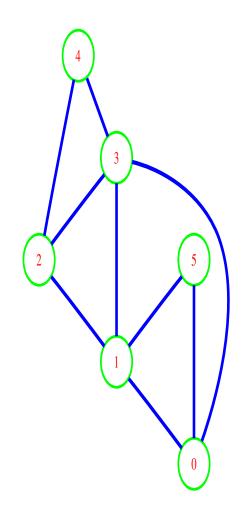


- ★ Cambridge-Ipswich high-tech corridor
- ★ 2000 technologists
- ★ 15 companies
- ★ UCL, Univ of Essex

Talk outline

- \star graph concepts and problems
- ★ chromatic number and clique number
- \star relaxations and optimization formulations
- ★ performance in practice
- \star random k-sat
- \star Hamiltonian paths

★ theme - Never mind the theory - how do things work in practice?



Graphs concepts

- ★ *clique* a complete subgraph
- ★ maximal clique a clique that cannot be extended to a larger one
- *lonely set* a pairwise disjoint set of nodes (stable set, independent set)
- ★ colouring an assignment of colours to nodes in which no neighbours have the same colour
- \star chromatic number χ the number of colours in a colouring with a minimal number of colours
- \star loneliness α the number of nodes in a largest lonely set
- ★ clique number ω the number of nodes in a largest maximal clique

Hard graph problems

\star finding χ , α and ω is proven to be NP-complete

this means that it unlikely that any algorithm exists which runs in time which is a polynomial function of the number of nodes

\star we therefore have two options:

▶ use a heuristic, which is probably fast but may give the wrong answer

- ▶ use an exact algorithm, and try to make it as fast as possible by clever coding
- ★ the theory is well developed and presented in many places, but little practical experience gets reported
- ★ therefore, I tried exact algorithms for these problems to determine how big the problems can be in practice, and compared the timings with approximate (relaxed) algorithms

Chromatic number χ

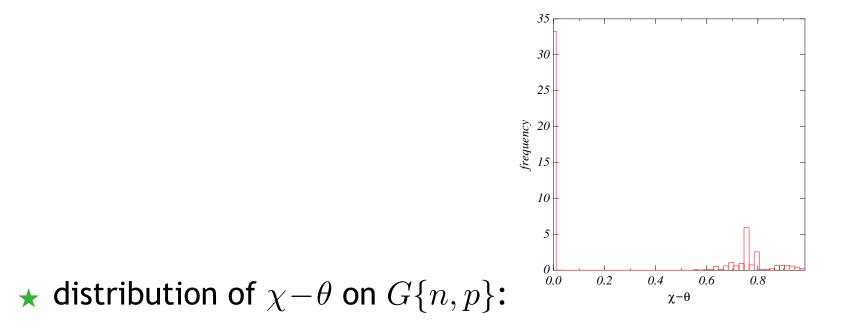
- many papers appeared in the 1980s about backtracking (branchand-bound) methods. Some had errors
 - idea: start to compute all colourings, but abort one as soon as it is worse than the best so far
- \star can be combined with heuristics (greedy colourings) and exact bounds like $\omega \leqslant \chi \leqslant \Delta + 1$, where Δ is the maximum degree
- ★ tradeoff in using heuristics depends on type of graph
- ★ in practice (with a well-written C program), up to 100 nodes is ok, and up to 200 for very sparse or very dense graphs
- best results are in a PhD by Chiarandini (Darmstadt 2005)
 http://www.imada.sdu.dk/~marco/public.php
- \star determining χ may be easy for many real-world graphs with specific structures (Coudert, DAC97)

Loneliness number α and clique number ω

- ★ best algorithm I found was one by Tsukiyama, Ide, Ariyoshi, & Shirakawa (SIAM J. Computing 6 505-517 (1977))
- \star can use graph complementation to flip these two calculations
- ★ in practice (with a well-written C program), up to 100 nodes is ok, and up to 200 for very sparse or very dense graphs

Relaxations and semidefinite programming

- ★ idea: formulate as an integer linear program (still hard), then relax constraints to obtain a semidefinite program (SDP, easy to solve)
- * SDP: provides the Lovász θ number for a graph. This number is an upper bound for the clique number of a graph, and a lower bound for the chromatic number
- * best SDP code: DSDP5.8 by Benson
 http://www-unix.mcs.anl.gov/DSDP/



LP formulation of chromatic number and clique number

- ★ let B be the 0-1 matrix with n rows and whose columns indicate the lonely sets (in practice, ok to use only maximal lonely sets). Finding B is slow
- \star chromatic number χ is the solution of the 0-1 ILP

 $\begin{array}{ll} \text{minimize} & \mathbf{1}^T x\\ \text{subject to} & Bx \geqslant 1 \end{array}$

 \star clique number ω is the solution of the 0-1 ILP

maximize $y^T 1$ subject to $y^T B \leqslant 1$

 \star solving the 0-1 ILPs is hard, so we don't try

Fractional chromatic number χ_{f}

- ★ used by McDiarmid for a radio channel assignment problem in which the demand (required number of channels) at each node varies
- $\star \chi_{\rm f}$ is the solution of the LP (ordinary LP, so easy)

 $\begin{array}{ll} \text{minimize} & \mathbf{1}^T x\\ \text{subject to} & Bx \geqslant 1\\ & x \geqslant 0 \end{array}$

 $\star \omega_{\rm f}$ is the solution of the LP (ordinary LP, so easy)

$$\begin{array}{ll} \mbox{maximize} & y^T 1 \\ \mbox{subject to} & y^T B \leqslant 1 \\ & y \geqslant 0 \end{array}$$

Typical results

\star I have programmed all the methods

graph	n	$p \operatorname{or} m$	lpha	ω	χ_{f}	χ	heta	
g1	10	0.5	4	4	4	4	4	medium
g2	10	0.9	3	7	7	7	7	dense
g3	10	0.1	9	2	2	2	2	sparse
g4	50	5	45	2	2	2	2	sparse, big
g5	50	100	23	3	3	3	3	medium density, big
gб	50	1000	4	14	16.5	17	15.36	high density, big

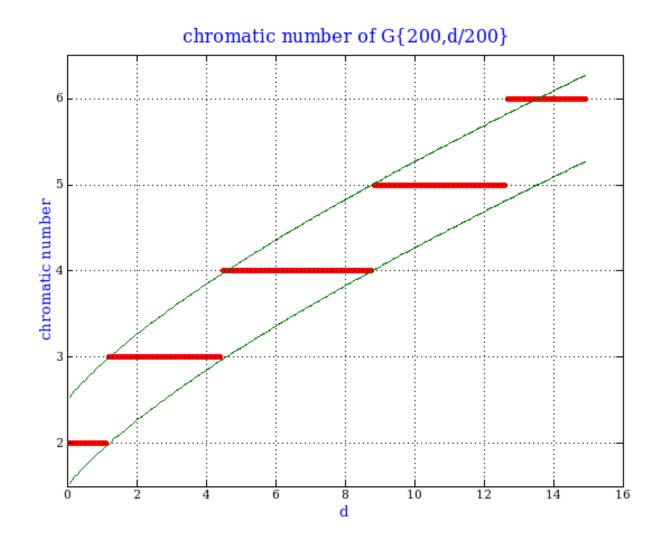
★ theorem: we always have $\omega \leq \omega_{f} \leq \chi_{f} \leq \chi$

★ recall $\omega \leq \theta \leq \chi$

Achlioptas & Naor

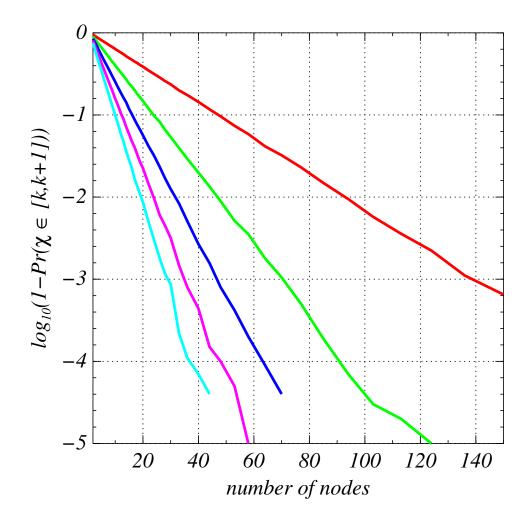
- ★ The two possible values of the chromatic number of a random graph Annals of Mathematics, 162 (2005) http://www.cs.ucsc.edu/~optas/
- ★ the authors show that for fixed d, as $n \to \infty$, the chromatic number of $G\{n, d/n\}$ is either k or k+1, where k is the smallest integer such that $d < 2k \log(k)$. In fact, this means that k is given by $\lceil d/(2W(d/2)) \rceil$
- \star $G\{n,p\}$ means the random graph on n nodes and each possible edge appears independently with probability p

Achlioptas & Naor cotd.



Achlioptas & Naor - my conjecture

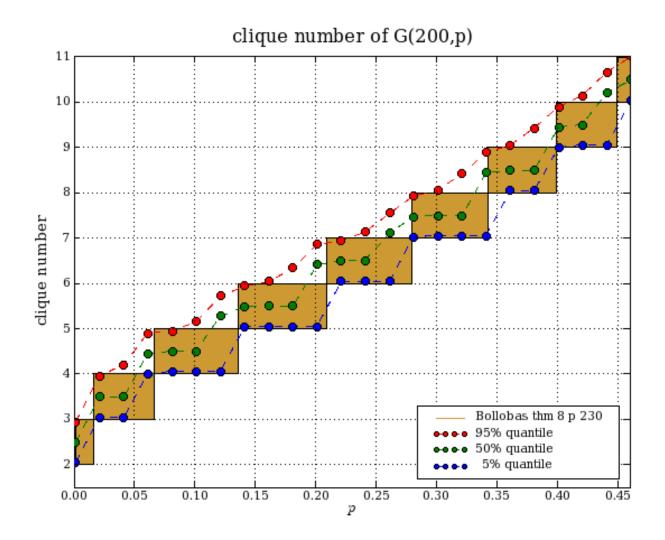
★ the next graph (each point is the average of 1 million trials) suggests that for small d, we have $\Pr[\chi \in [k, k+1]] \sim 1 - \exp(-dn/2)$



Cliques

- ★ In Modern graph theory, page 230, Bollobás shows that the clique number of G(n,p) as $n \to \infty$ is almost surely d or d+1, where d is the greatest natural number such that $\binom{n}{d}p^{\binom{d}{2}} \ge \log(n)$
- \star How accurate is this formula when n is small?
- * We have $d = 2\log(n)/\log(1/p) + \mathcal{O}(\log\log(n))$.

Cliques - simulation results



Counting graphs

Number of graphs on n nodes with chromatic number k:

n =	1	2	3	4	5	6	7	8	9	10	
k											
2	0	1	2	6	12	34	87	302	1118	5478	A076278
3	0	0	1	3	16	84	579	5721	87381	2104349	A076279
4	0	0	0	1	4	31	318	5366	155291	7855628	A076280
5	0	0	0	0	1	5	52	867	28722	1919895	A076281
6	0	0	0	0	0	1	6	81	2028	115391	A076282
7	0	0	0	0	0	0	1	7	118	4251	
8	0	0	0	0	0	0	0	1	8	165	
9	0	0	0	0	0	0	0	0	1	9	
10	0	0	0	0	0	0	0	0	0	1	
11	0	0	0	0	0	0	0	0	0	0	

(A-numbers from http://www.research.att.com/~njas/sequences/)

Counting graphs cotd.

Number of graphs on n nodes with clique number k:

n =	1	2	3	4	5	6	7	8	9	10	
k											
2	0	1	2	6	13	37	106	409	1896	12171	A052450
3	0	0	1	3	15	82	578	6021	101267	2882460	A052451
4	0	0	0	1	4	30	301	4985	142276	7269487	A052452
5	0	0	0	0	1	5	51	842	27107	1724440	A077392
6	0	0	0	0	0	1	6	80	1995	112225	A077393
7	0	0	0	0	0	0	1	7	117	4210	A077394
8	0	0	0	0	0	0	0	1	8	164	
9	0	0	0	0	0	0	0	0	1	9	
10	0	0	0	0	0	0	0	0	0	1	

(A-numbers from http://www.research.att.com/~njas/sequences/)

Another NP-complete problem: *k*-sat

- \star *n* Boolean variables
- \bigstar Boolean function f in CNF: consists of the "and" (\land) of a number of clauses
- \star each clause is the "or" (\lor) of k variables or their negations

 $\star \text{ e.g. } f(x) = (x_1 \lor x_2 \lor x_3) \land (x_1 \lor x_2 \lor \overline{x_3}) \land (x_1 \lor \overline{x_2} \lor x_3) \land (\overline{x_1} \lor x_2 \lor x_3)$

- \star k-sat: find an assignment x of the variables such that f(x) = 1
- * useful for finding feasible points in scheduling problems etc.
- \star hard to find a solution, easy to verify a proposed solution
- \star 2-sat is easy, k-sat for k > 3 can be reduced to 3-sat
- \star therefore, we can use heuristics to find solutions

Random *k*-sat

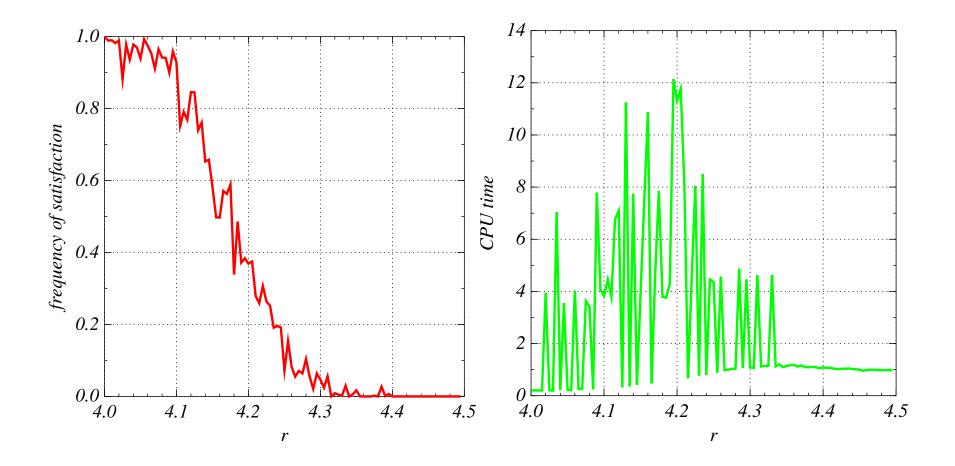
- \star choose clauses randomly, with r being the ratio of the number of clauses to the number of variables
- * recent (2002) big breakthrough: survey propagation by Mézard, Parisi & Zecchina (http://www.sciencemag.org/cgi/content/ abstract/297/5582/812 and many other articles in Nature and Science): physics-inspired heuristic that works (at least for random 3-sat) even for $n > 10^5$

> my experience: works worse than other heuristics on small, structured problems

 \star there is a phase transition near $r_{\rm c} = 4.26$, where random 3-sat jumps from being almost surely satisfiable to almost surely unsatisfiable

Random 3-sat phase transition

 \star I computed this with the survey propagation heuristic - 1000 variables x_i , 100 trials for each value of r:



Hamiltonian path problem

- \star find a path in a graph that visits every node once and only once
- ★ NP-complete
- ★ can encode as a k-sat problem (Knuth Boolean Basics problem 40 - errors!) and use heuristic
- \star let p_{uv} mean u < v in a ordering of the nodes, and let q_{uvw} mean u < v < w
- ★ they express the constraints that consecutive nodes are adjacent (i.e. non-adjacent nodes (~) are non-consecutive)
- ★ the graph has a Hamiltonian path iff the set of clauses on the next page is satisfiable
- ★ recall that $(\overline{x} \lor y) \equiv (x \Rightarrow y)$
- \star can we do Hamiltonian circuits this way?

Hamiltonian path encoding

 $\star p_{uv} \lor p_{vu}$ for all pairs $u \neq v$ (i.e. either u < v or v < u)

 $\star \ \overline{p}_{uv} \vee \overline{p}_{vu}$ for all pairs $u \neq v$ (i.e. not both u < v and v < u)

- $\label{eq:puv} \star \ \overline{p}_{uv} \lor \overline{p}_{vw} \lor p_{uw} \ \text{for all pairs} \ u \neq v, u \neq w, v \neq w \\ \text{(i.e. } u < v \ \text{and} \ v < w \Rightarrow u < w \text{)}$
- $\star \overline{q}_{uvw} \lor p_{uv}$ for $u \not\sim w$ (i.e. $u < v < w \Rightarrow u < v$)
- $\star \overline{q}_{uvw} \lor p_{vw}$ for $u \nsim w$ (i.e. $u < v < w \Rightarrow v < w$)
- $\star q_{uvw} \lor \overline{p}_{uv} \lor \overline{p}_{vw}$ (i.e. $\overline{u < v < w} \Rightarrow u > v$ or v > w)
- $\star q_{uvw} \lor q_{wvu}$ for $u \nsim w$ and $\forall v \notin \{u, w\}$
- ★ I wrote a python program to translate any given graph into these clauses and solve them with a satisfier
- ★ http://www.research.att.com/~njas/sequences/A115065

The future

- ★ work on making the practical algorithms faster, by using more efficient data structures etc.
- \star understand the accuracy of the θ bound
- \star what is the distribution of $\theta-\chi$ for standard ensembles of random graphs?
- ★ study properties of special graphs arising in real applications scale-free, unit-disk etc.
- \star understand the k-sat phase transition
- \star encode more real problems as k-sat
- ★ see the book Perfect graphs (ed. J L Ramírez Alfonsín & B A Reed) for lots more on applications to networks