# Some practical experiences <br> of <br> hard graph problems 

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## BT Research at Martlesham, Suffolk


$\star \begin{aligned} & \text { Cambridge-Ipswich } \\ & \text { high-tech corridor }\end{aligned}$
$\star 2000$ technologists
$\star 15$ companies
$\star$ UCL, Univ of Essex

## Talk outline

* graph concepts and problems
* chromatic number and clique number
$\star$ relaxations and optimization formulations
* performance in practice
* random $k$-sat
* Hamiltonian paths
* theme - Never mind the theory - how do things work in practice?


## Graphs concepts


$\star$ 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 $\chi$ - the number of colours in a colouring with a minimal number of colours
$\star$ loneliness $\alpha$ - the number of nodes in a largest lonely set
* clique number $\omega$ - the number of nodes in a largest maximal clique


## Hard graph problems

* finding $\chi, \alpha$ and $\omega$ is proven to be NP-complete
$\triangleright$ this means that it unlikely that any algorithm exists which runs in time which is a polynomial function of the number of nodes
* we therefore have two options:
$\triangleright$ use a heuristic, which is probably fast but may give the wrong answer
$\triangleright$ 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 $\chi$

* many papers appeared in the 1980s about backtracking (branch-and-bound) methods. Some had errors
$\triangleright$ idea: start to compute all colourings, but abort one as soon as it is worse than the best so far
* can be combined with heuristics (greedy colourings) and exact bounds like $\omega \leqslant \chi \leqslant \Delta+1$, where $\Delta$ 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
$\star$ best results are in a PhD by Chiarandini (Darmstadt 2005) http://www.imada.sdu.dk/~marco/public.php
* determining $\chi$ may be easy for many real-world graphs with specific structures (Coudert, DAC97)


## Loneliness number $\alpha$ and clique number $\omega$

* best algorithm I found was one by Tsukiyama, Ide, Ariyoshi, \& Shirakawa (SIAM J. Computing 6 505-517 (1977))
* 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 $\theta$ 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/
* distribution of $\chi-\theta$ on $G\{n, p\}$ :


LP formulation of chromatic number and clique number
$\star$ 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

* chromatic number $\chi$ is the solution of the 0-1 ILP

$$
\begin{array}{rc}
\text { minimize } & 1^{T} x \\
\text { subject to } & B x \geqslant 1
\end{array}
$$

* clique number $\omega$ is the solution of the 0-1 ILP

| maximize | $y^{T} 1$ |
| ---: | :---: |
| subject to | $y^{T} B \leqslant 1$ |

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


## Fractional chromatic number $\chi_{\mathrm{f}}$

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

$$
\begin{array}{cc}
\text { minimize } & 1^{T} x \\
\text { subject to } & B x \geqslant 1 \\
& x \geqslant 0
\end{array}
$$

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

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

## Typical results

* I have programmed all the methods

| graph | $n$ | $p$ or $m$ | $\alpha$ | $\omega$ | $\chi_{\mathrm{f}}$ | $\chi$ | $\theta$ |  |
| :---: | :---: | :---: | ---: | ---: | ---: | ---: | ---: | :--- |
| 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 |
| g6 | 50 | 1000 | 4 | 14 | 16.5 | 17 | 15.36 | high density, big |

* theorem: we always have $\omega \leqslant \omega_{\mathrm{f}} \leqslant \chi_{\mathrm{f}} \leqslant \chi$
$\star$ recall $\omega \leqslant \theta \leqslant \chi$


## 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 $n \rightarrow \infty$, the chromatic number of $G\{n, d / n\}$ is either $k$ or $k+1$, where $k$ is the smallest integer such that $d<2 k \log (k)$. In fact, this means that $k$ is given by $\lceil d /(2 W(d / 2))\rceil$
$\star G\{n, p\}$ 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 $\operatorname{Pr}[\chi \in[k, k+1]] \sim 1-\exp (-d n / 2)$



## Cliques

* In Modern graph theory, page 230, Bollobás shows that the clique number of $G(n, p)$ as $n \rightarrow \infty$ is almost surely $d$ or $d+1$, where $d$ is the greatest natural number such that $\binom{n}{d} p^{\binom{d}{2}} \geqslant \log (n)$
* How accurate is this formula when $n$ is small?
$\star$ 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 $k$ :

| $\mathrm{n}=$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 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 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 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

* $n$ Boolean variables
* Boolean function $f$ in CNF: consists of the "and" ( $\wedge$ ) of a number of clauses
* each clause is the "or" $(\vee)$ of $k$ variables or their negations
$\star$ e.g. $f(x)=\left(x_{1} \vee x_{2} \vee x_{3}\right) \wedge\left(x_{1} \vee x_{2} \vee \overline{x_{3}}\right) \wedge\left(x_{1} \vee \overline{x_{2}} \vee x_{3}\right) \wedge\left(\overline{x_{1}} \vee x_{2} \vee x_{3}\right)$
$\star k$-sat: find an assignment $x$ of the variables such that $f(x)=1$
* useful for finding feasible points in scheduling problems etc.
* hard to find a solution, easy to verify a proposed solution
* 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

* 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 $n>10^{5}$
$\triangleright$ my experience: works worse than other heuristics on small, structured problems
* there is a phase transition near $r_{\mathrm{c}}=4.26$, where random 3 -sat jumps from being almost surely satisfiable to almost surely unsatisfiable


## Random 3-sat phase transition

* I computed this with the survey propagation heuristic - 1000 variables $x_{i}$, 100 trials for each value of $r$ :




## Hamiltonian path problem

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


## Hamiltonian path encoding

$\star p_{u v} \vee p_{v u}$ for all pairs $u \neq v$ (i.e. either $u<v$ or $v<u$ )
$\star \bar{p}_{u v} \vee \bar{p}_{v u}$ for all pairs $u \neq v$ (i.e. not both $u<v$ and $v<u$ )
$\star \bar{p}_{u v} \vee \bar{p}_{v w} \vee p_{u w}$ for all pairs $u \neq v, u \neq w, v \neq w$
(i.e. $u<v$ and $v<w \Rightarrow u<w$ )
$\star \bar{q}_{u v w} \vee p_{u v}$ for $u \nsim w($ i.e. $u<v<w \Rightarrow u<v$ )
$\star \bar{q}_{u v w} \vee p_{v w}$ for $u \nsim w($ i.e. $u<v<w \Rightarrow v<w$ )
$\star q_{u v w} \vee \bar{p}_{u v} \vee \bar{p}_{v w}$ (i.e. $\overline{u<v<w} \Rightarrow u>v$ or $v>w$ )
$\star q_{u v w} \vee q_{w v u}$ 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.

夫 understand the accuracy of the $\theta$ bound

* 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.
* understand the $k$-sat phase transition
* 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

