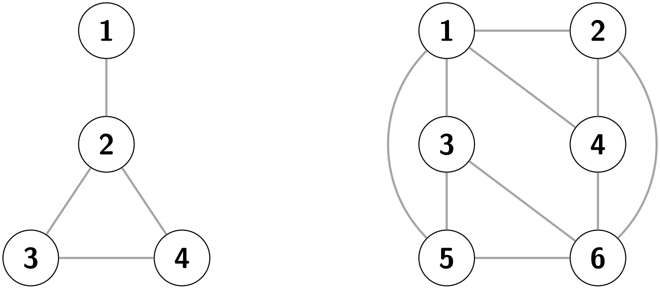
Subgraph Isomorphism in Practice

Ciaran McCreesh, Patrick Prosser and James Trimble

Non-Induced Subgraph Isomorphism



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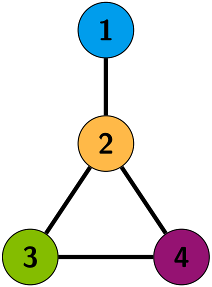
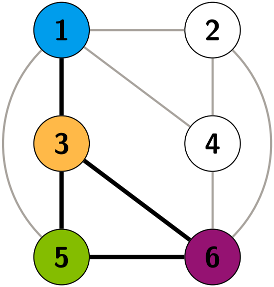




The Algorithm

- Recursively build up a mapping from vertices of the pattern graph to vertices of the target graph.
- In constraint programming terms:
  - Forward-checking recursive search.
  - A variable for every pattern vertex.
  - Initially, each domain contains every target vertex.
  - After guessed assignments, infeasible values are eliminated from domains.
    - All-different constraint.
    - Adjacency constraints.
  - If we get a wipeout, we backtrack.

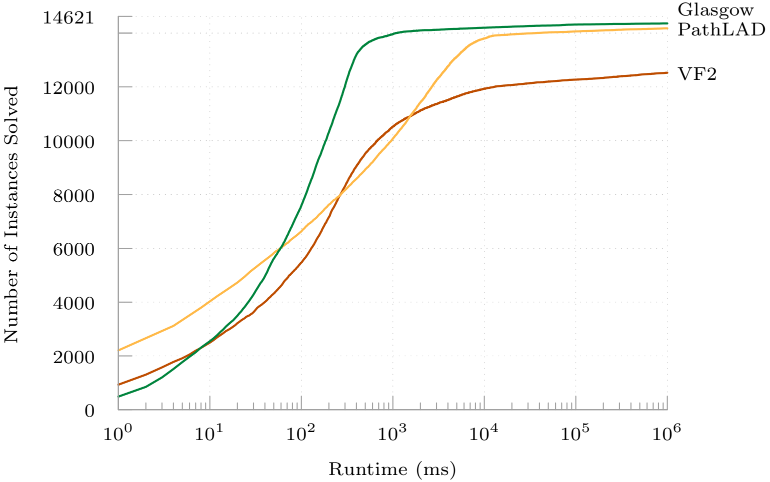
But wait! There's more!

- Clever filtering at the top of search using neighbourhood degree sequences and paths, to reduce the initial values of domains.
- Pre-computed path count constraints, propagated like adjacency constraints during search.
- Bit-parallel implementation.
  - Weaker than the usual all-different propagator, but much faster.

Benchmark Instances

- 14,621 instances from Christine Solnon's collection:
  - Randomly generated with different models.
  - Real-world graphs.
  - Computer vision problems.
  - Biochemistry problems.
  - Phase transition instances.
- At least...
  - $\geq 2,110$ satisfiable.
  - $\geq 12,322$ unsatisfiable.
- A lot of them are very easy for good algorithms.

Is It Any Good?



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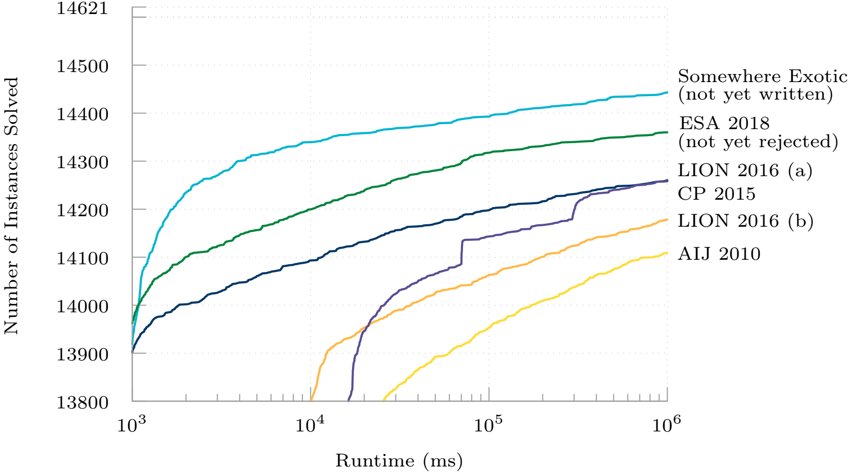


Search Order

- Variable ordering (i.e. pattern vertices): smallest domain first, tie-breaking on highest degree.
- Value ordering (i.e. target vertices): highest degree to lowest.

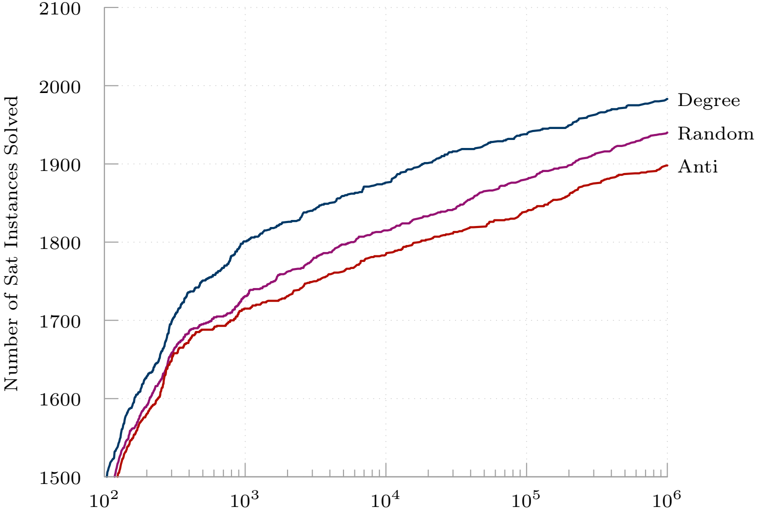
Hand-Wavy Theoretical Justification

- Maximise the expected number of solutions during search?
- If $P = G(p, q)$ and $T = G(t, u)$,

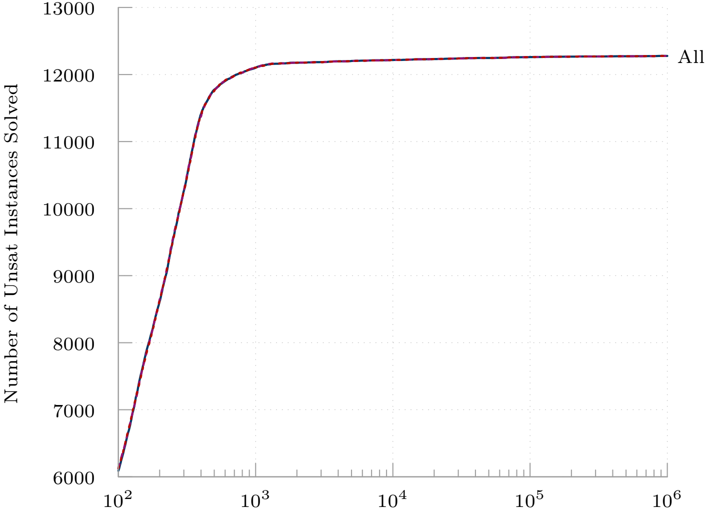
$$\langle Sol \rangle = \underbrace{t \cdot (t-1) \cdot \ldots \cdot (t-p+1)}_{\text{injective mapping}} \cdot \underbrace{u^{q \cdot \binom{p}{2}}}_{\text{adjacency}}$$

- Smallest domain first keeps remaining domain sizes large.
- High pattern degree makes the remaining pattern subgraph sparser, reducing q.
- High target degree leaves as many vertices as possible available for future use, making u larger.

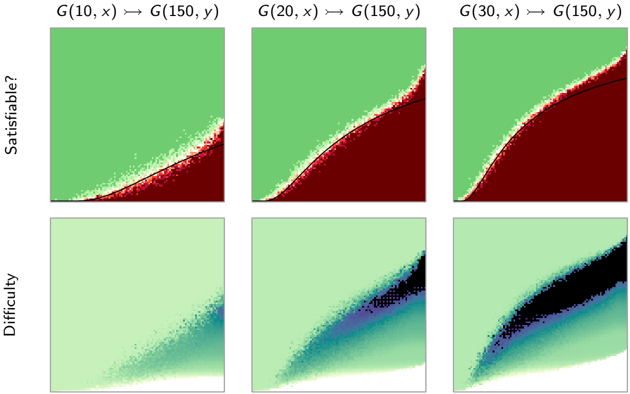
Sanity Check



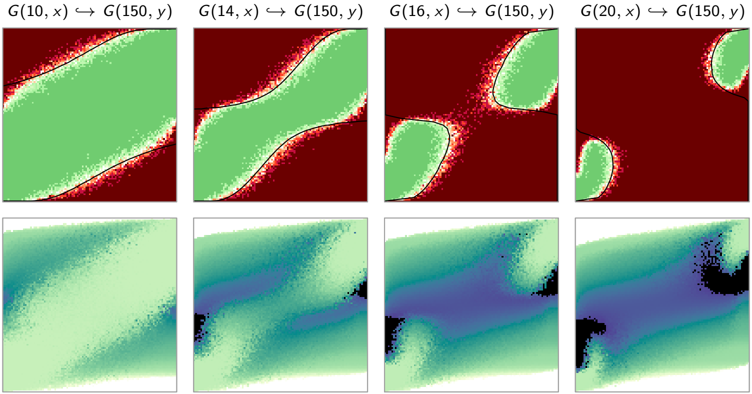
Sanity Check



Phase Transitions



Incidentally, Induced is Much More Complicated



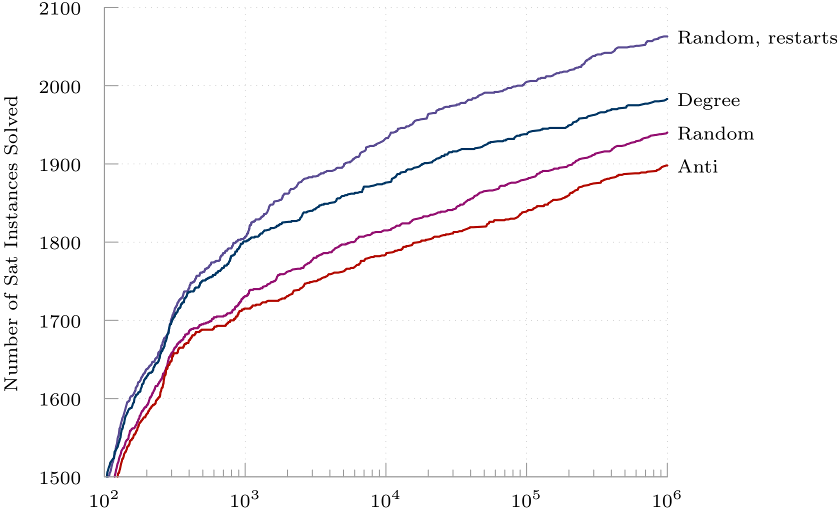
However. . .

- Degree spread is low.
- We commit extremely heavily to the first branching choice, which is probably wrong.

Restarts

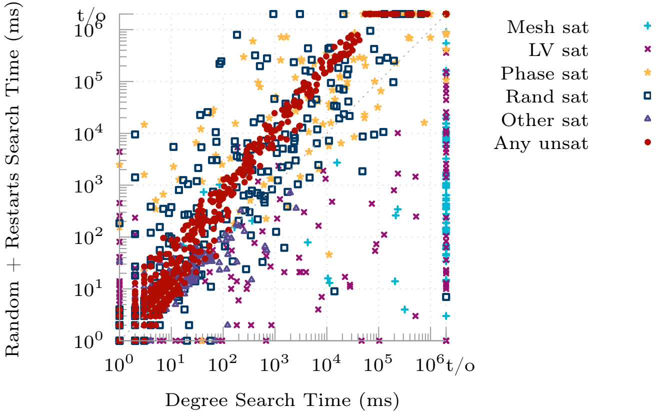
- Run search for a bit, and if we don't find a solution, restart.
- Count number of backtracks, restart using the Luby sequence (with a magic constant multiplier).
  - 1, 1, 2, 1, 1, 2, 4, 1, 1, 2, 1, 1, 2, 4, 8, . . .
- Obviously, something needs to change when we restart.
  - First attempt: random value-ordering heuristic.

Restarts



2100
2000
1900
1800
1700
1600
1500
Number of Sat Instances Solved
10^2
10^3
10^4
10^5
10^6
Random, restarts
Degree
Random
Anti

Restarts



Random + Restarts Search Time (ms)
Degree Search Time (ms)
t/o
10^0 10^1 10^2 10^3 10^4 10^5 10^6
Mesh sat
LV sat
Phase sat
Rand sat
Other sat
Any unsat

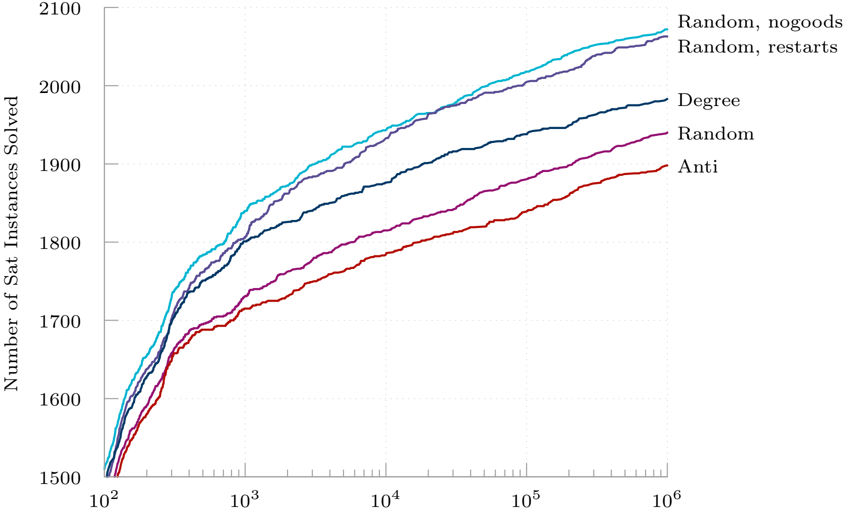
Nogoods

- Whenever we restart, post new constraints eliminating parts of the search space already explored.
- Potentially exponentially many constraints.
- But they are all in the form

$$(d_1 = v_1) \wedge (d_2 = v_2) \wedge \ldots \wedge (d_n = v_n) \to \bot.$$

- Use two watched literals to propagate in $O(1)$ish time.
  - Basic idea: clauses only propagate when exactly one $(d_i = v_i)$ literal has not been set to true.
  - Watch *two* literals per clause that have not been set to true.
  - When unit propagating, only look at clauses with a watch corresponding to the assignment made.
  - Either find a new literal to watch, or propagate.

Nogoods



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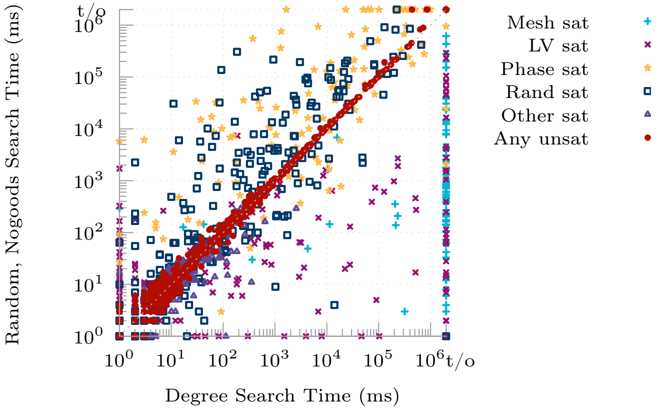
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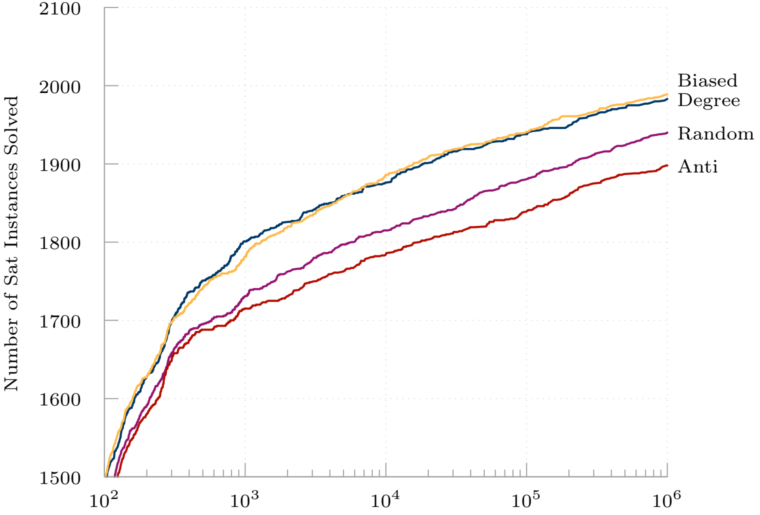
Biased Value-Ordering

- Select a vertex v' from the chosen domain D_v with probability

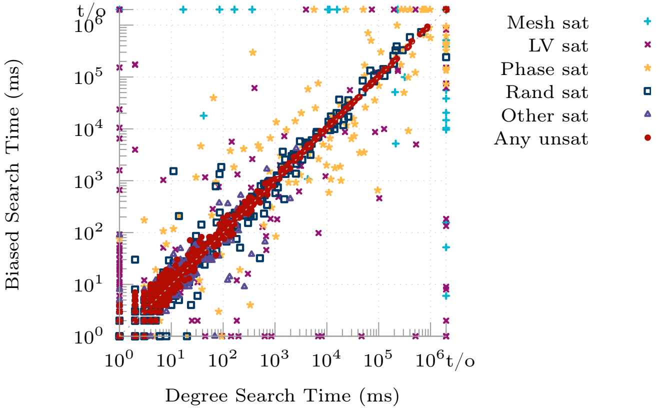
$$p(v') = \frac{2^{\deg(v')}}{\sum_{w \in D_v} 2^{\deg(w)}}.$$

- Looks a lot like *softmax*, which uses base e.

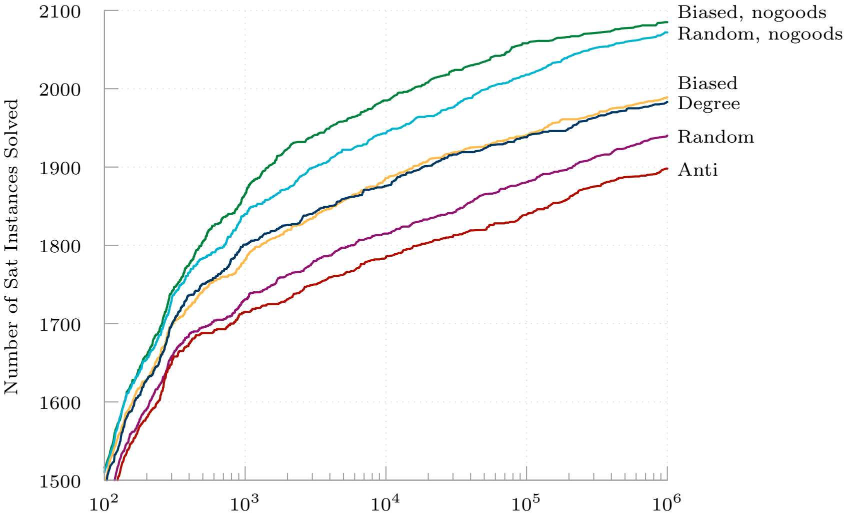
Biased Value-Ordering



Biased Value-Ordering



Biased Value-Ordering with Restarts and Nogoods



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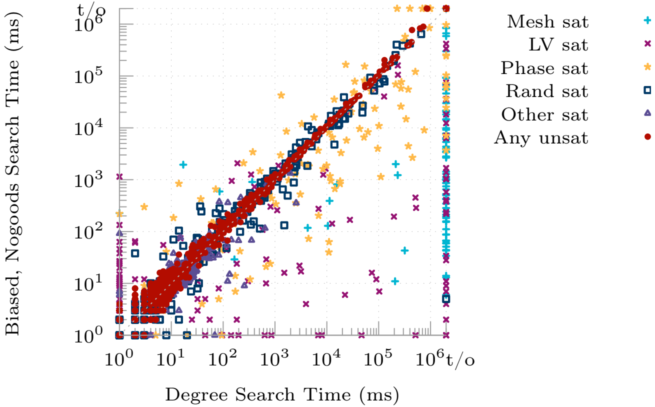

Ongoing Work

- Is this form of search more broadly applicable?
- Specialisations, like clique, and generalisations, like maximum common subgraph.
- Parallelism.
- Subgraphs modulo theories.
- Algorithm engineering.

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