Finding Little Graphs Inside Big Graphs

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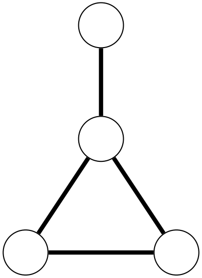
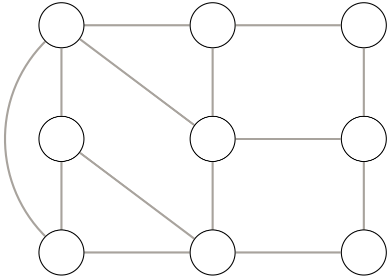
Subgraph Isomorphism





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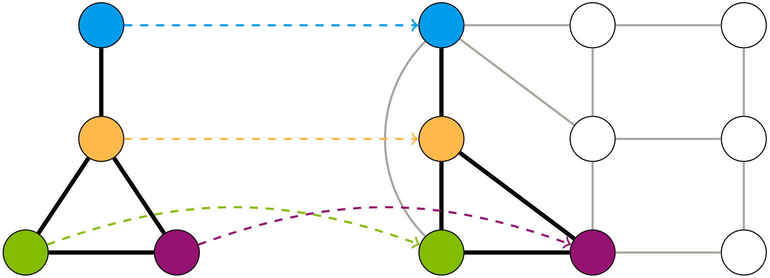

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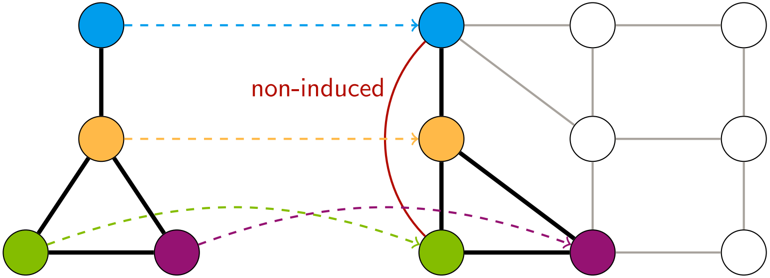

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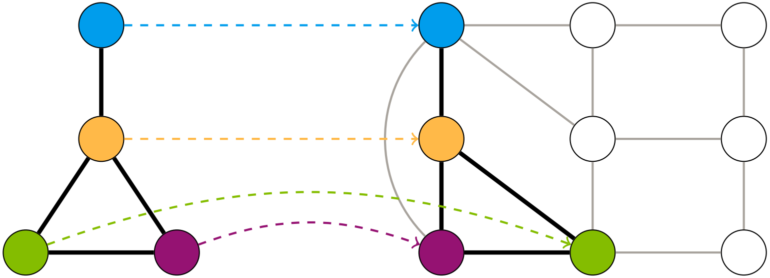

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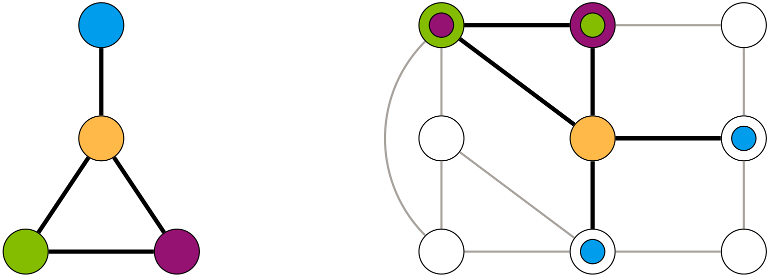

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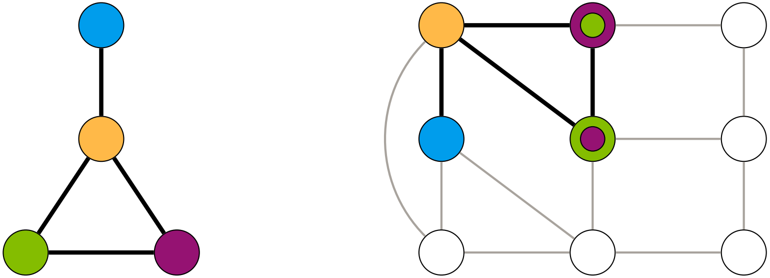

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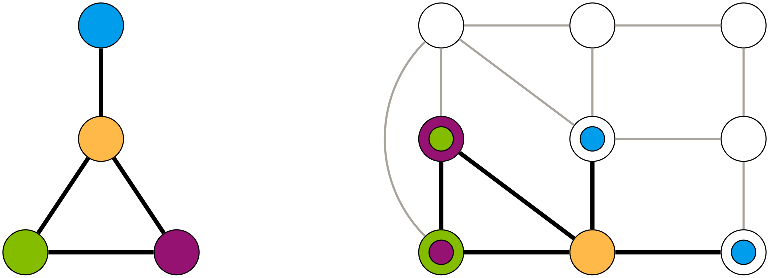

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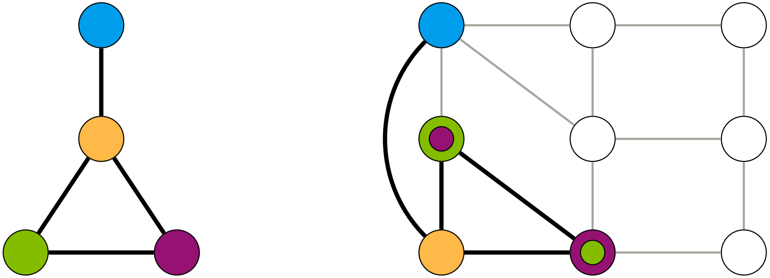

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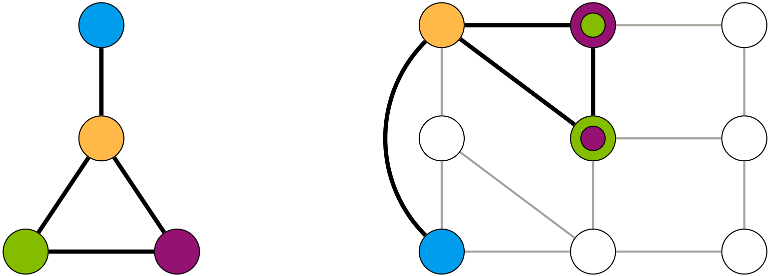
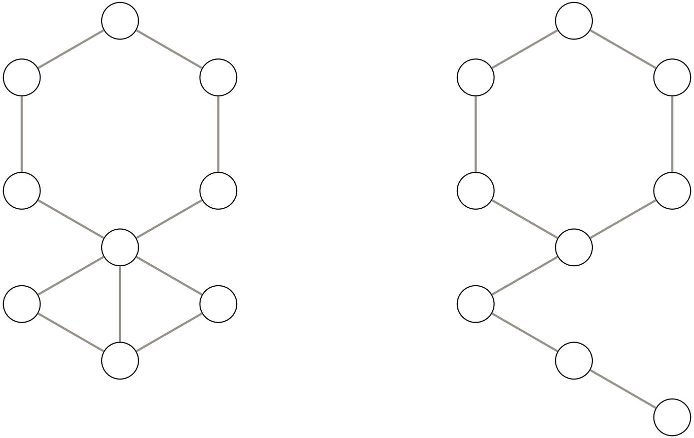


Maximum Common Induced Subgraph



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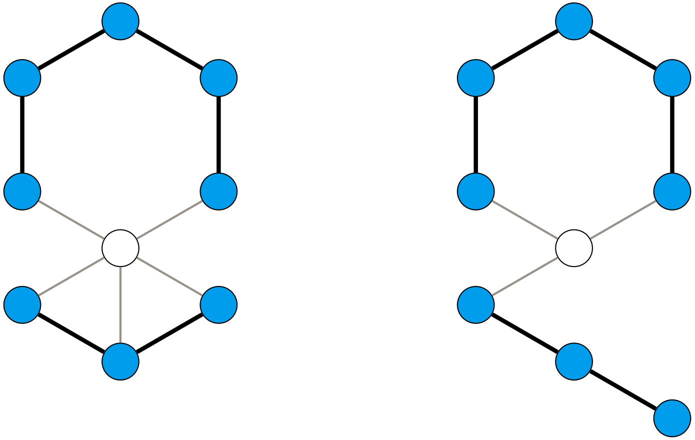
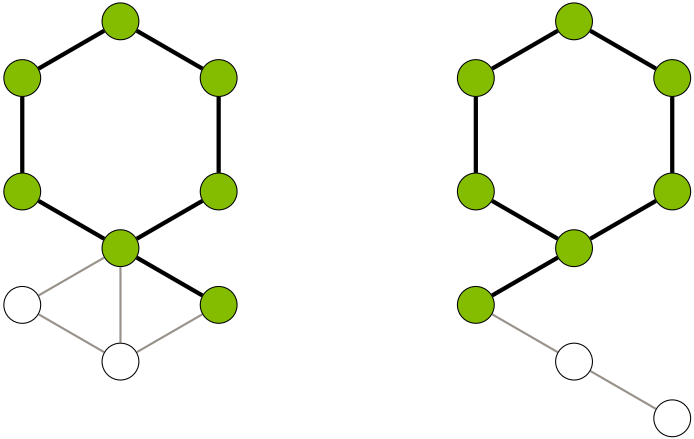
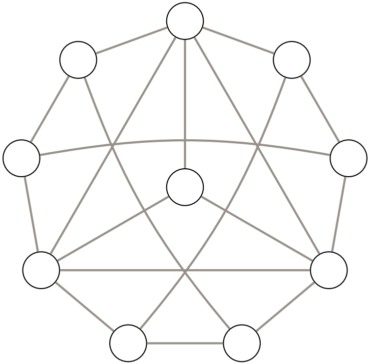


Maximum Common Induced Connected Subgraph



Maximum Clique



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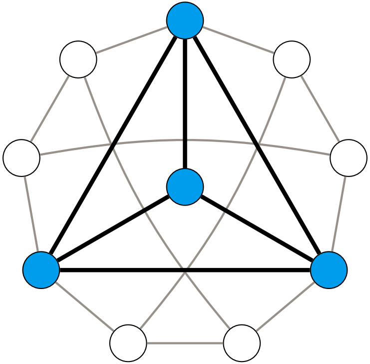

Who Cares?

- Chemistry, biochemistry, and drug design (graphs are molecule fragments or proteins).
- Computer vision.
- Compilers (instruction generation, code rewriting).
- Plagiarism and malware detection.
- Livestock epidemiology (contact and trade graphs).
- Designing mechanical lock systems.

In Theory. . .

- Subgraph finding is hard.
- Subgraph counting is hard.
- Approximate subgraph finding is hard.

In Practice. . .

- We have good *solvers* for subgraph problems.
- Some applications involve solving thousands of subgraph isomorphism queries per second.
- We can solve clique on larger graphs than we can solve all-pairs shortest path.[1]

[1] Terms and conditions apply.

In Practice. . .

- We have good *solvers* for subgraph problems.
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In Practice. . .

- We have good *solvers* for subgraph problems.
- Some applications involve solving thousands of subgraph isomorphism queries per second.
- We can solve clique on larger graphs than we can solve all-pairs shortest path.[1]
- Maximum common subgraph is still a nightmare. . .
- People often don't actually want to solve simple subgraph isomorphism.

[1] Terms and conditions apply.

Graphs Aren't Just Graphs

- Vertex and / or edge labels, or broader compatibility functions.
- Directed edges.
- Multi-edges, more than one edge between vertices.
- Hyper-edges, between more than two vertices.
- Partially defined graphs?
- No need for injectivity (homomorphism), or only local injectivity.

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- Don't forget about loops!
- Might want all solutions, or a count.

Two Solver Design Philosophies

1. Pick a vertex, guess where it goes, and start trying to grow a connected component.
   - Popular solvers: VF2, VF3, RI, TurboISO, . . .
   - Very fast to start up.
   - Often good on easy instances.
   - Spectacularly bad on hard instances, and on some easy instances.
2. Use constraint programming, build a mapping from the pattern graph to the target graph.
   - LAD, Glasgow Subgraph Solver.
   - Consistent performance on easy instances.
   - Much better on hard instances.

The Glasgow Subgraph Solver

`https://github.com/ciaranm/glasgow-subgraph-solver`

- A CP style solver specifically for subgraph algorithms.
- Subgraph isomorphism, and all its variants (induced / non-induced, homomorphism, locally injective, labels, side constraints, directed, . . .).
- Also special algorithms for clique.
- Guaranteed no bugs!

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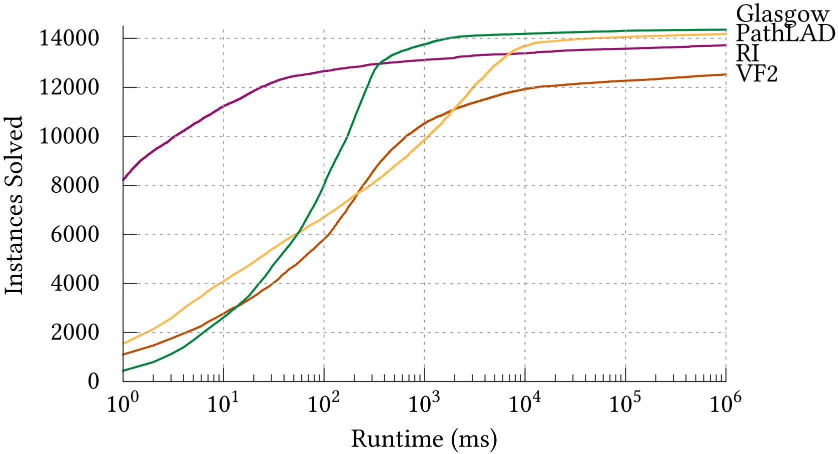
- Also special algorithms for clique.
- Guaranteed no bugs!
  - Or at least, any buggy output will always be detected, if you enable proof logging.

Benchmark Instances

http://perso.citi-lab.fr/csolnon/SIP.html

- 14,621 instances from Christine Solnon's collection:
  - Randomly generated with different models (MIVIA suite).
  - 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?



Easy Conclusion!

- CP is best!

An Observation about Certain Datasets

- All of the randomly generated instances from the MIVIA suites are satisfiable.
- The target graphs are randomly generated, and patterns are made by selecting random connected subgraphs and permuting them.
- These instances are usually rather easy. . .
- Many papers use *only* these instances for benchmarking.

A Different Easy Conclusion!

- CP is slow! RI is best!

Constraint Programming

- We have some variables, each of which has a domain of possible values.
- Give each variable a value from its domain, whilst respecting all constraints.

Building a Mapping

- One variable per pattern vertex.
- Domains and values are target vertices.
- We think of these variables as defining a function.

Injectivity

- Can't map to the same target vertex twice.
- Could say that each pair of pattern vertices are not equal?

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- Can't map to the same target vertex twice.
- Could say that each pair of pattern vertices are not equal?
- We prefer high-level constraints, so we just say "all different".

Adjacency

- If A and B are adjacent in the pattern, $f(A)$ must be adjacent to $f(B)$ in the target.
- Various ways of encoding this. In SAT we'd need n^4 clauses, or n^3 if we're sneaky.
- In practice: we write a special constraint propagator to do this efficiently.

Backtracking Search, Maintaining Consistency

- Pick a variable V that has more than one value remaining.
- For each of its values v in turn:
  - Try $V = v$, and do some inference.
    - No other variable can take the value v.
    - Variables adjacent to V must be given values adjacent to v.
  - If we get an empty domain, we made a bad guess.
  - If every variable has one value left, we have a solution.
  - Otherwise, recurse.

Data Structures

- We store a set of values for every variable.
- Need to be able to test whether a specific value is present, remove values, count how many values remain.
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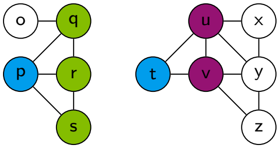
- Must either be copyable, or have some way of doing backtracking.
- Objectively correct answer: bitsets.

Degree Filtering

- Can't map a vertex of degree d to a vertex of degree less than d.



Neighbourhood Degree Sequences

- Can't map a vertex whose neighbours have degree 4, 3, 2 to a vertex whose neighbours have degree 4, 2, 2, 2.

Dynamic Degrees?

- If a target vertex disappears from every domain, can pretend it's not there at all.
- This reduces the degree of all of its neighbours.
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- Maybe this leads to more filtering?
- Problem: detecting this can be moderately expensive, so possibly not worth doing?

Adjacency Filtering

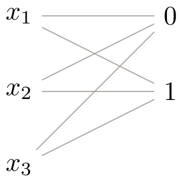
- When P gets mapped to t, neighbours of P can only be mapped to neighbours of t.
- Store domains and neighbourhoods as bitsets.

Injectivity Filtering

$$A \in \{1, 2\}$$
$$B \in \{2, 3\}$$
$$C \in \{1, 3\}$$
$$D \in \{1, 4, 5, 6\}$$
$$E \in \{2, 5\}$$
$$F \in \{3, 5\}$$

Matchings and All-Different

- Draw a vertex on the left for each variable, and a vertex on the right for each value.
- Draw edges from each variable to each of its values.
- A *maximum cardinality matching* is where you pick as many edges as possible, but each vertex can only be used at most once.
- We can find this in polynomial time.
- There is a matching which covers each variable if and only if the constraint can be satisfied.
- In fact, there is a one to one correspondence between perfect matchings and solutions to the constraint.



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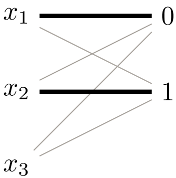

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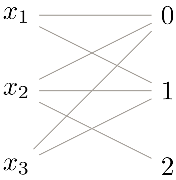

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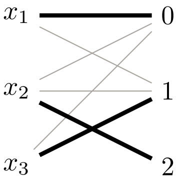

Sudoku

From Wikipedia, the free encyclopedia

Not to be confused with Sodoku or Sudeki.

Sudoku (数独 *sūdoku*?, digit-single) /suːˈdoʊkuː/, /-ˈdɒ-/, /sə-/; originally called **Number Place**,[1] is a logic-based,[2][3] combinatorial[4] number-placement puzzle. The objective is to fill a 9×9 grid with digits so that each column, each row, and each of the nine 3×3 sub-grids that compose the grid (also called "boxes", "blocks", "regions", or "sub-squares") contains all of the digits from 1 to 9. The puzzle setter provides a partially completed grid, which for a well-posed puzzle has a unique solution.

5	3			7				
6			1	9	5			
	9	8					6	
8				6				3
4			8		3			1
7				2				6
	6					2	8	
			4	1	9			5
				8			7	9

A typical Sudoku puzzle

5	3	4	6	7	8	9	1	2
6	7	2	1	9	5	3	4	8
1	9	8	3	4	2	5	6	7
8	5	9	7	6	1	4	2	3
4	2	6	8	5	3	7	9	1
7	1	3	9	2	4	8	5	6
9	6	1	5	3	7	2	8	4
2	8	7	4	1	9	6	3	5
3	4	5	2	8	6	1	7	9

The same puzzle with solution numbers marked in red

How do Humans Solve Sudoku?

18	23	23	245	456	456	279	378	23589

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How do Humans Solve Sudoku?

1	23	23	245	456	456	279	378	23589

How do Humans Solve Sudoku?

1	23	23	245	456	456	279	378	23589

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1	23	23	245	456	456	279	378	23589

How do Humans Solve Sudoku?

1	23	23	245	456	456	279	378	23589

How do Humans Solve Sudoku?

1	23	23	45	456	456	79	78	589

How do Humans Solve Sudoku?

1	23	23	45	456	456	79	78	589

How do Humans Solve Sudoku?

1	23	23	45	456	456	79	78	589

How do Humans Solve Sudoku?

1	23	23	45	456	456	79	78	89

Generalised Arc Consistency

- Arc Consistency (AC): for a binary constraint, each value is supported by at least one value in the other variable.
- Generalised Arc Consistency (GAC): for a global constraint, we can pick any value from any variable, and find a supporting set of values from each other variable in the constraint simultaneously.
  - Each remaining value appears in at least one solution to the constraint.

Hall Sets

- A *Hall set* of size n is a set of n variables from an "all different" constraint, whose domains have n values between them.
- If we can find a Hall set, we can safely remove these values from the domains of every other variable involved in the constraint.
- Hall's Marriage Theorem: doing this is equivalent to deleting every edge from the matching graph which cannot appear in any perfect matching.
- So, if we delete every Hall set, we delete every value that cannot appear in at least one way of satisfying the constraint. In other words, we obtain GAC.

GAC for All-Different

- There are 2^n potential Hall sets, so considering them all is probably a bad idea...
- Similarly, enumerating every perfect matching is #P-hard.
- However, there is a polynomial algorithm!

GAC for All-Different

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GAC for All-Different

18	23	23	245	456	456	279	378	23589

x_0

x_1

x_2

x_3

x_4

x_5

x_6

x_7

x_8

GAC for All-Different

18	23	23	245	456	456	279	378	23589

x_0	1
x_1	2
x_2	3
x_3	4
x_4	5
x_5	6
x_6	7
x_7	8
x_8	9

GAC for All-Different

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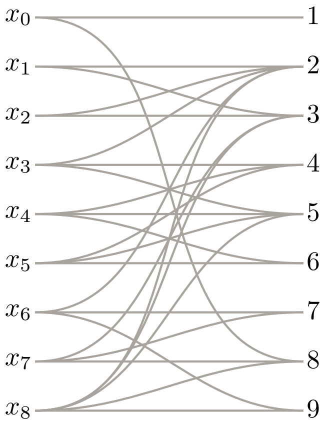

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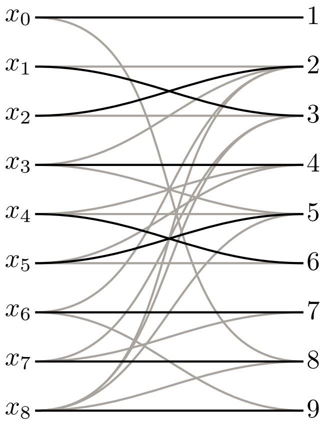

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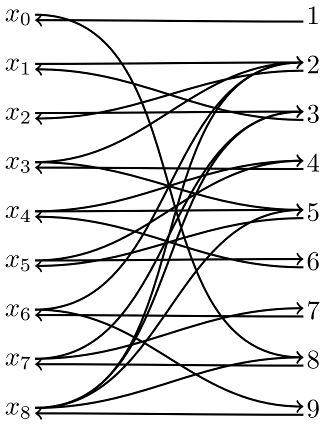

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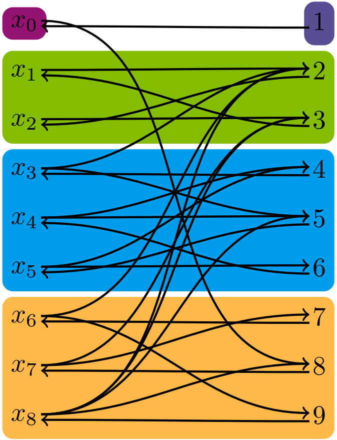

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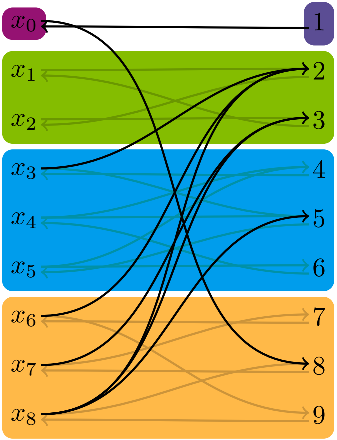

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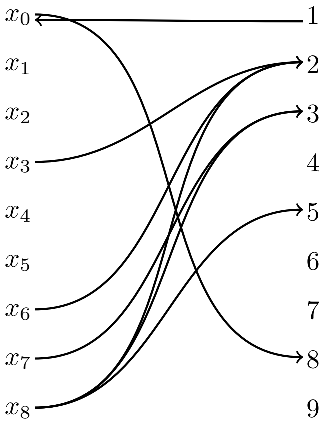

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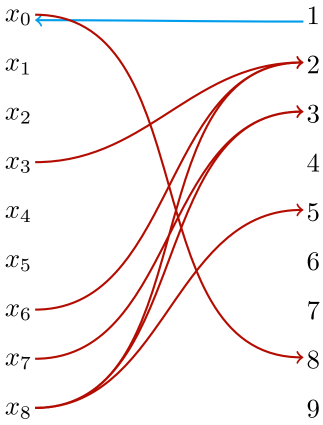

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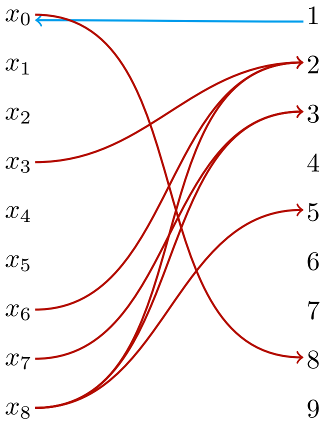

Is This a Good Idea?

- Various techniques to avoid running all-different all of the time.
  - Faster bit-parallel propagator that can miss some deletions.
- Can also do all-different on edges. . .

Distance Filtering

- Adjacent vertices must be mapped to adjacent vertices.

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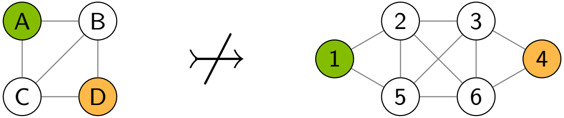
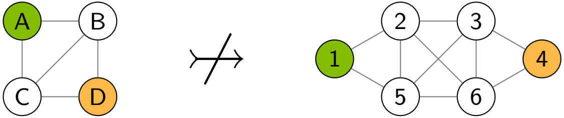
- Vertices that are distance 2 apart must be mapped to vertices that are within distance 2.



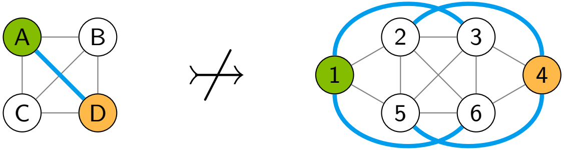
Distance Filtering

- Adjacent vertices must be mapped to adjacent vertices.
- Vertices that are distance 2 apart must be mapped to vertices that are within distance 2.
- Vertices that are distance k apart must be mapped to vertices that are within distance k.



Distance Filtering

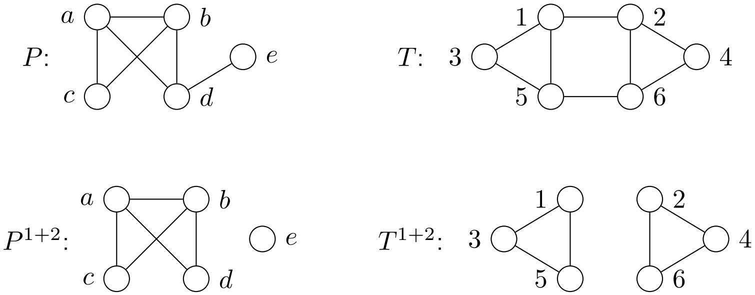
- G^d is the graph with the same vertex set as G, and an edge between v and w if the distance between v and w in G is at most d.
- For any d, a subgraph isomorphism $i : P \rightarrowtail T$ is also a subgraph isomorphism $i^d : P^d \rightarrowtail T^d$.



Distance Filtering

- We can do something stronger: rather than looking at distances, we can look at (simple) paths, and we can count how many there are.
- This is NP-hard in general, but only lengths 2 and 3 and counts of 2 and 3 are useful in practice.
- We construct these graph pairs once, at the top of search, and use them for degree-based filtering at the top of search, and “adjacency” filtering during search.

Supplemental Constraints



Induced Subisomorphisms

- Find something that is a non-induced subisomorphism

$$P \rightarrowtail T$$

and simultaneously a non-induced subisomorphism

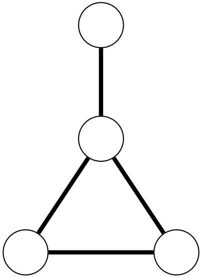
$$\overline{P} \rightarrowtail \overline{T}$$

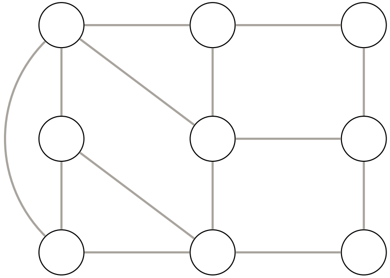
Partially Defined Graphs

- Challenge for you!

Clique Neighbourhood Filtering

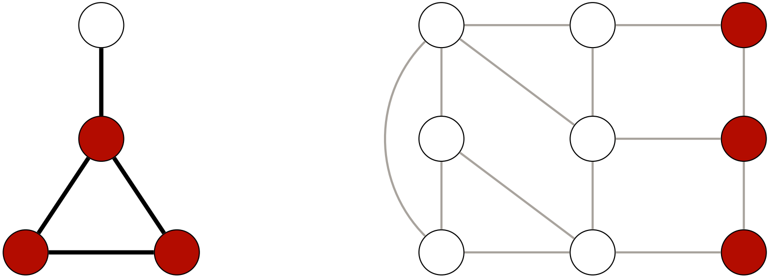
- If a pattern vertex is contained in a k-vertex clique, it must be mapped to a target vertex contained in at least a k-vertex clique.
- Valid without injectivity (with a caveat for loops).





Clique Neighbourhood Filtering

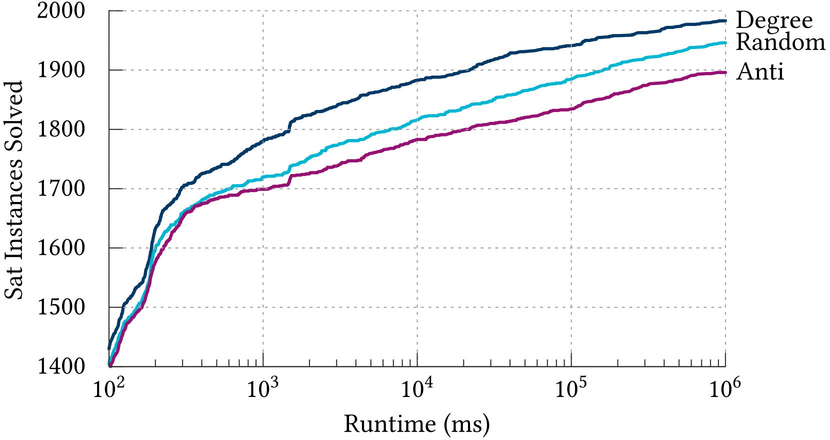
- If a pattern vertex is contained in a k-vertex clique, it must be mapped to a target vertex contained in at least a k-vertex clique.
- Valid without injectivity (with a caveat for loops).



Variable and Value Ordering Heuristics

- Variable ordering (i.e. pattern vertices): smallest domain first, tie-breaking on highest degree.
  - Tends to pick vertices adjacent to things we've already picked.
- Value ordering (i.e. target vertices): highest degree to lowest.

Sanity Check



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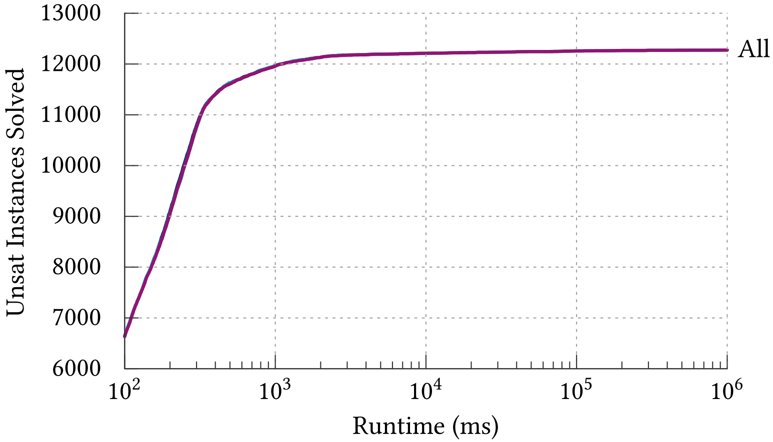
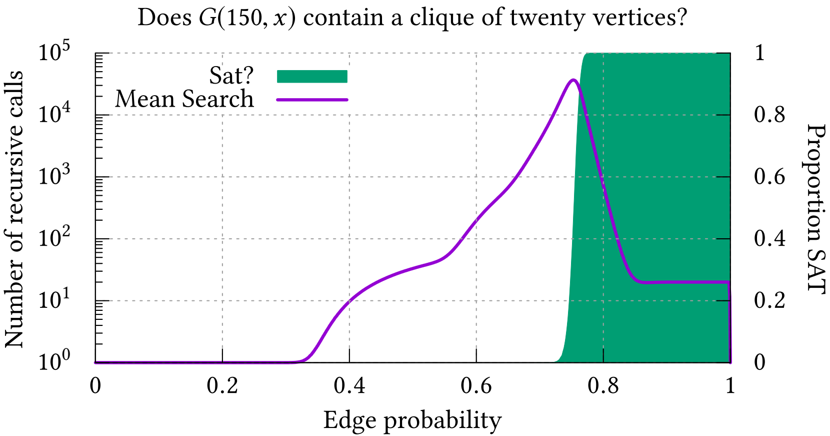


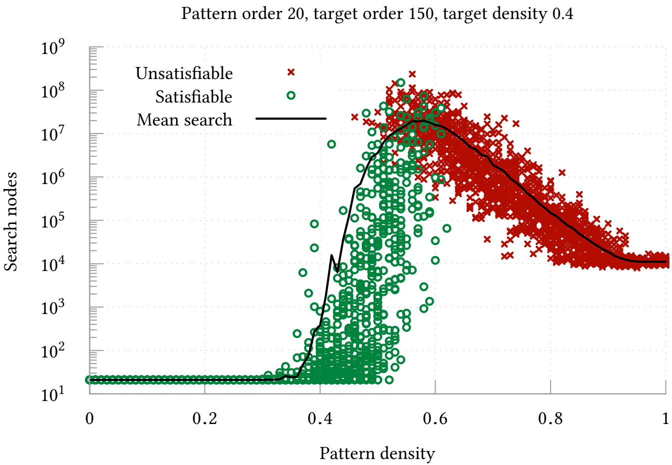
Clique in Random Graphs



Let's Generate Random Instances a Different Way

- Decide upon a pattern graph order (number of vertices) and density.
- Decide upon a target graph order and density.
- Generate instances at random, independently.

When is Non-Induced Subgraph Isomorphism Hard?



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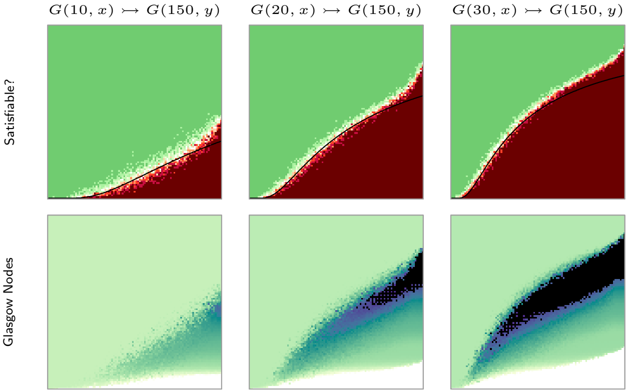

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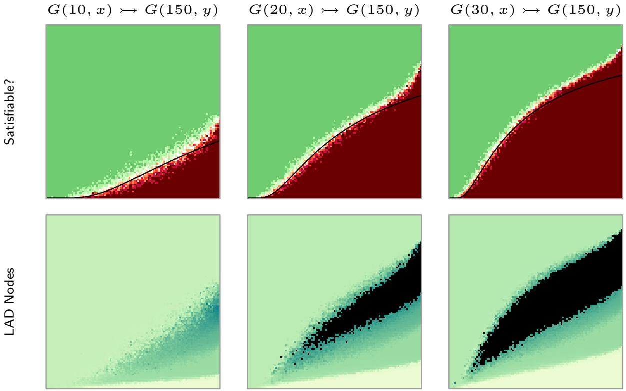

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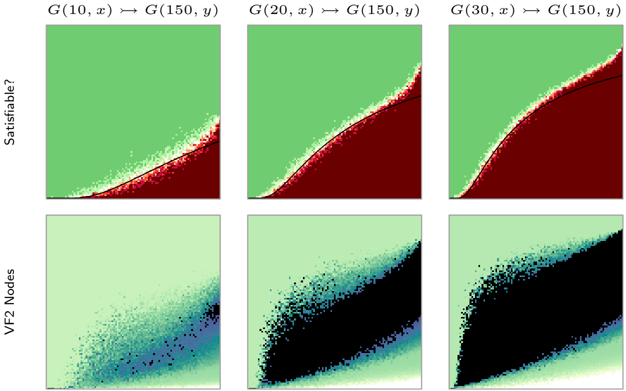


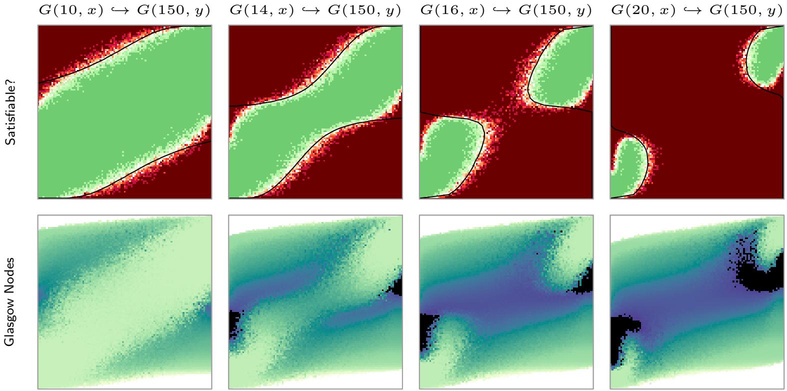
Hand-Wavy Theoretical Justification

- 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.

Induced is Much More Complicated



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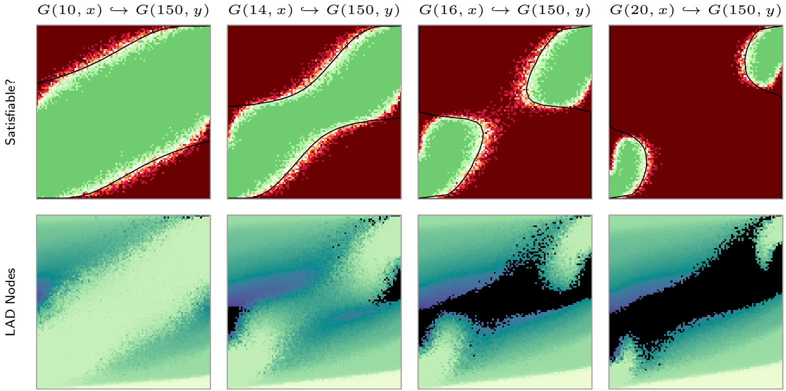

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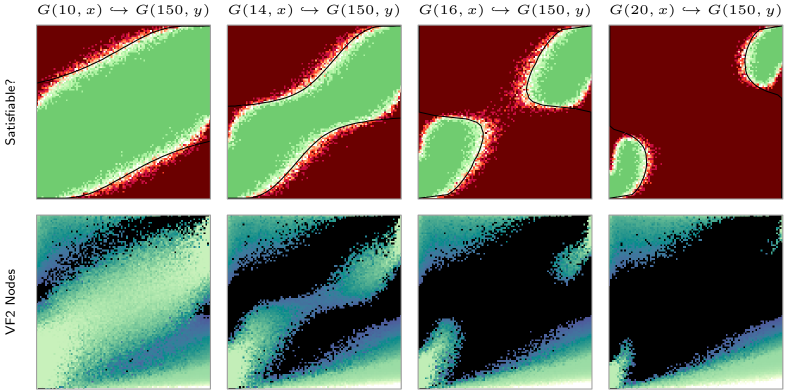

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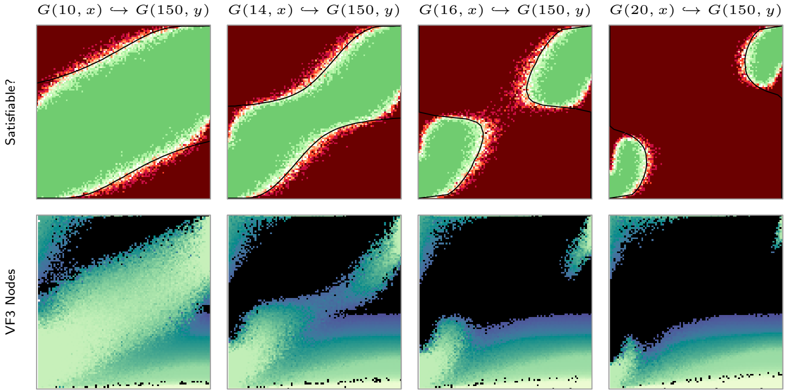
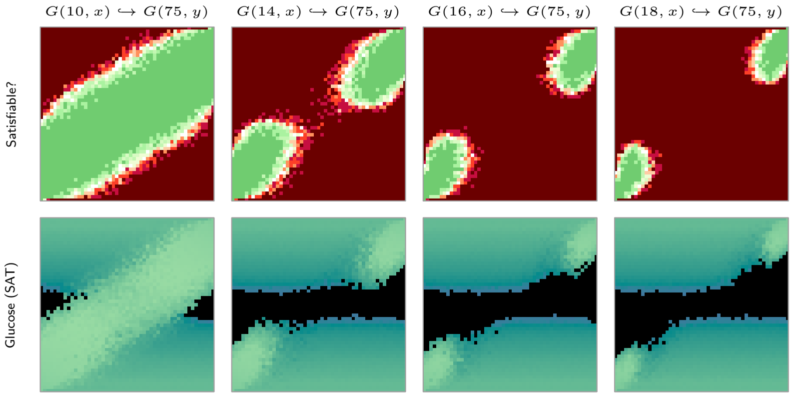


Is This Algorithm-Independent?



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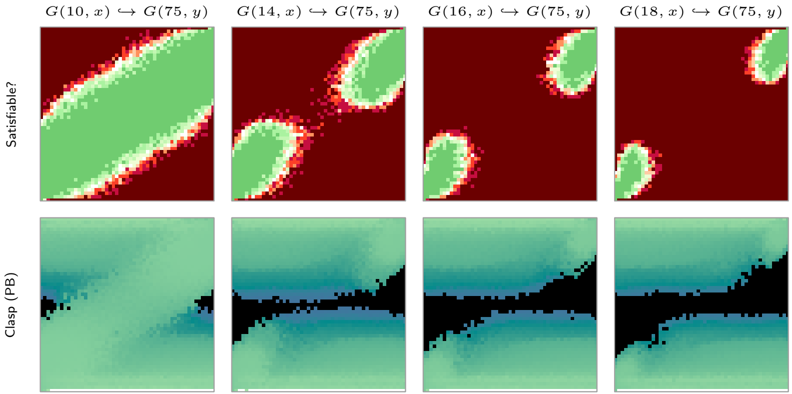

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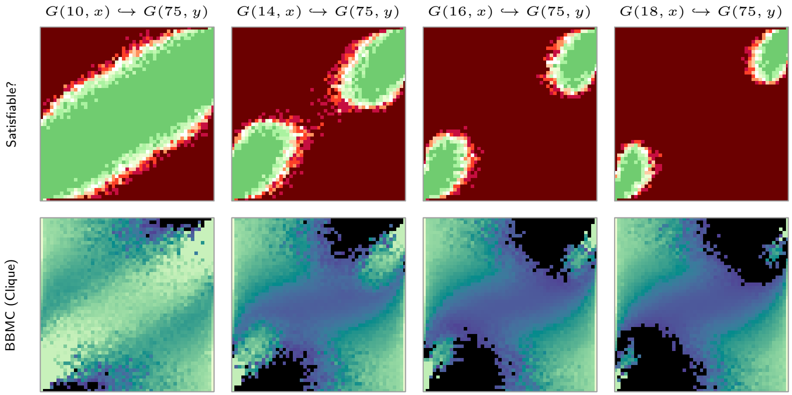

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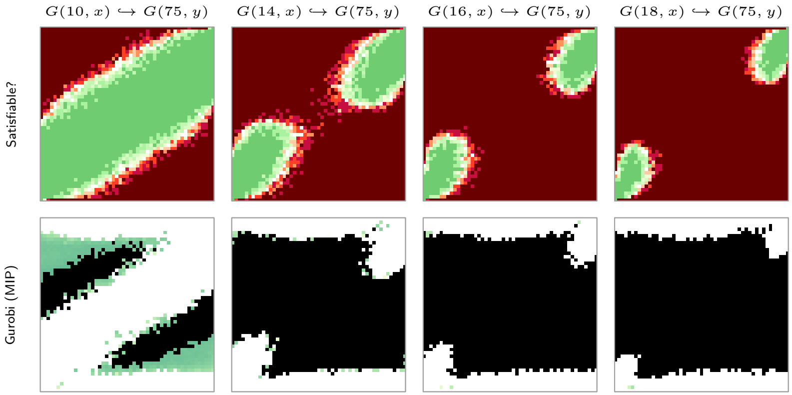
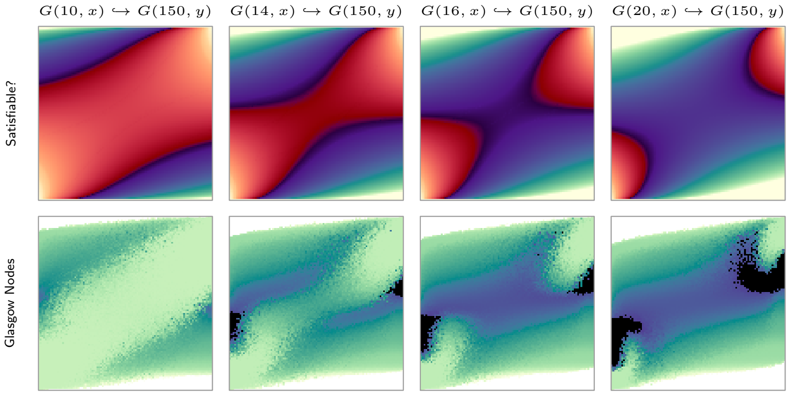


Constrainedness

$$\kappa = 1 - \frac{\log\left(t^{\underline{p}} \cdot u^{q \cdot \binom{p}{2}} \cdot (1-u)^{(1-q) \cdot \binom{p}{2}}\right)}{\log t^{\underline{p}}}$$

Constrainedness

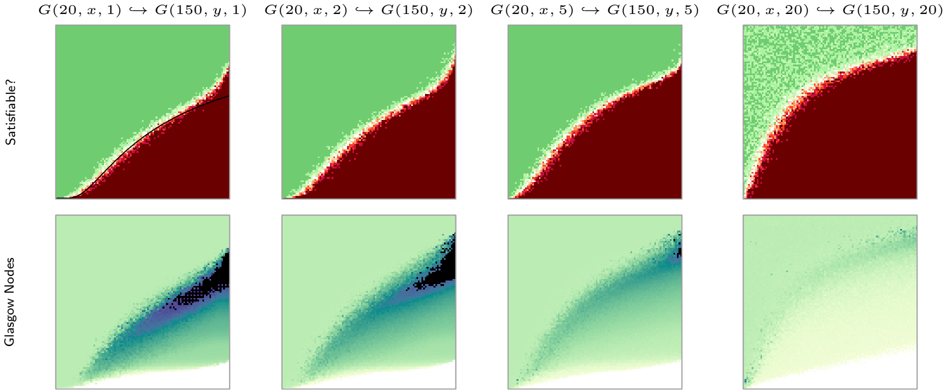


Labelled Subgraph Isomorphism

- Vertices have labels, and the isomorphism must preserve labels.
- Carbon must map to carbon, hydrogen to hydrogen, . . .

$$\langle Sol \rangle = \left(\frac{\Gamma\left({}^{t}\!/\!{}_{k} + 1\right)}{\Gamma\left({}^{t}\!/\!{}_{k} - {}^{p}\!/\!{}_{k} + 1\right)} \right)^{k} \cdot u^{q \cdot \binom{p}{2}}$$

Labels and Phase Transitions



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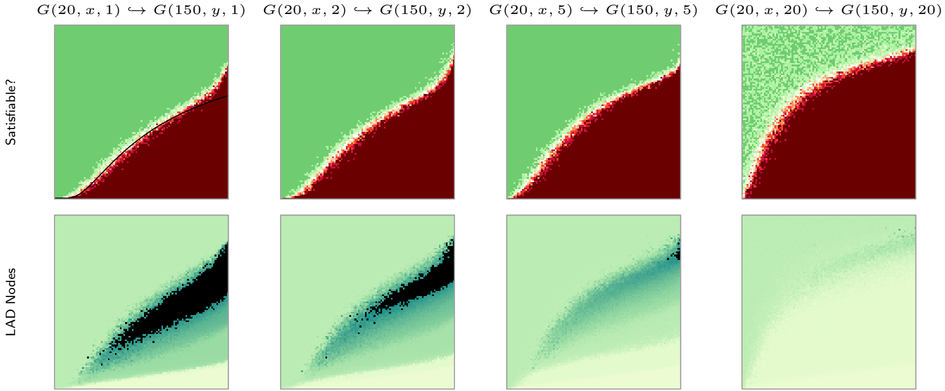

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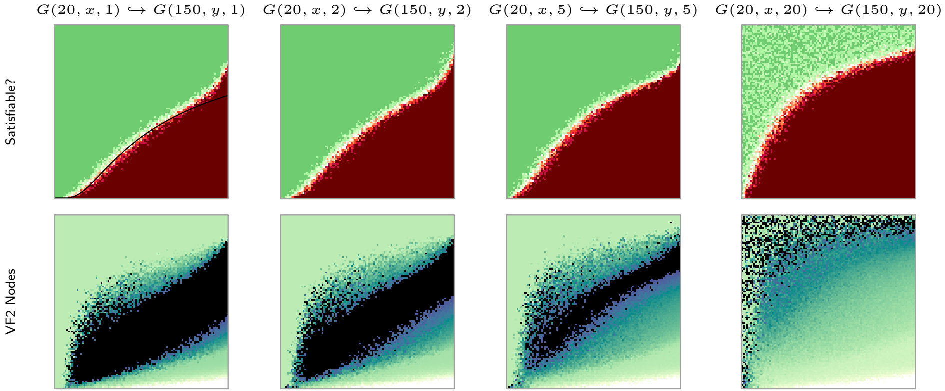
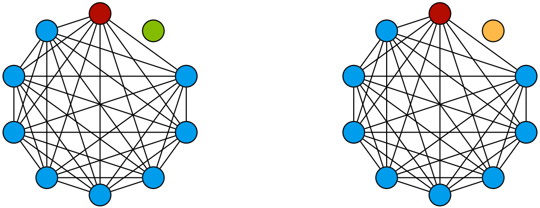


Connectivity Algorithms are Really Stupid



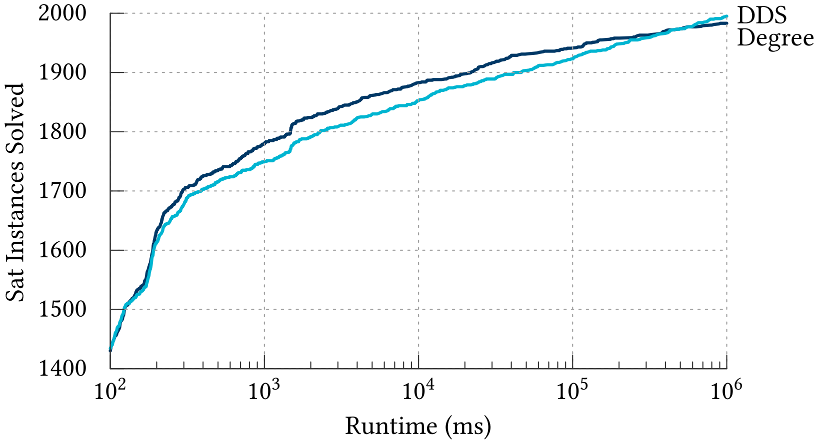
Back to Value-Ordering Heuristics

- Largest target degree first.

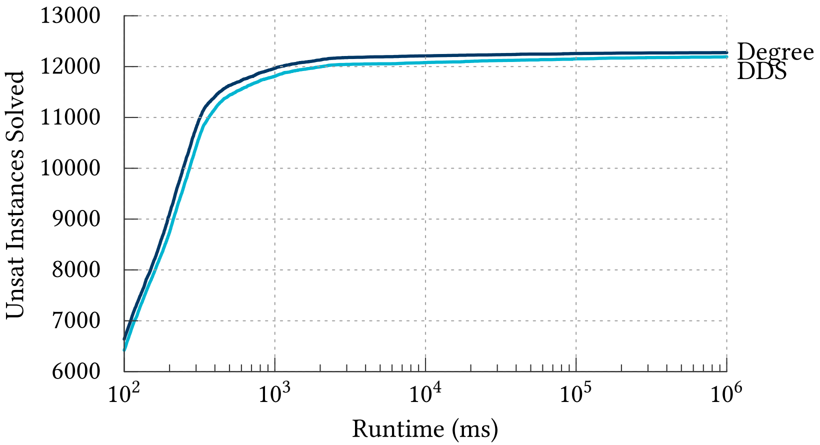
However. . .

- What if several vertices have the same degree?
- Is a vertex of degree 10 really that much better than a vertex of degree 9?

Discrepancy Search?



Discrepancy Search?



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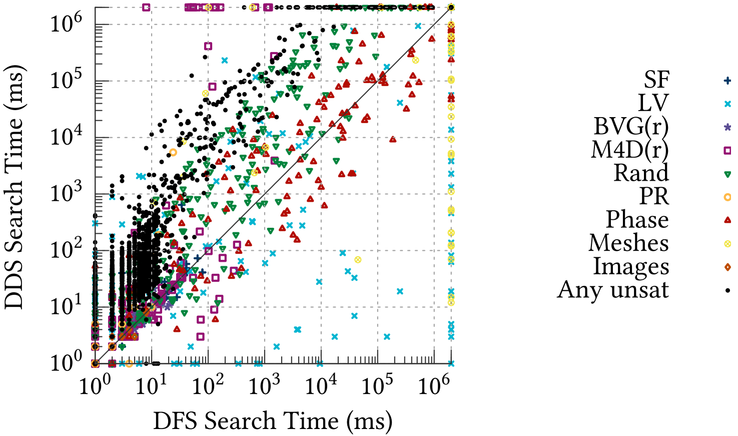
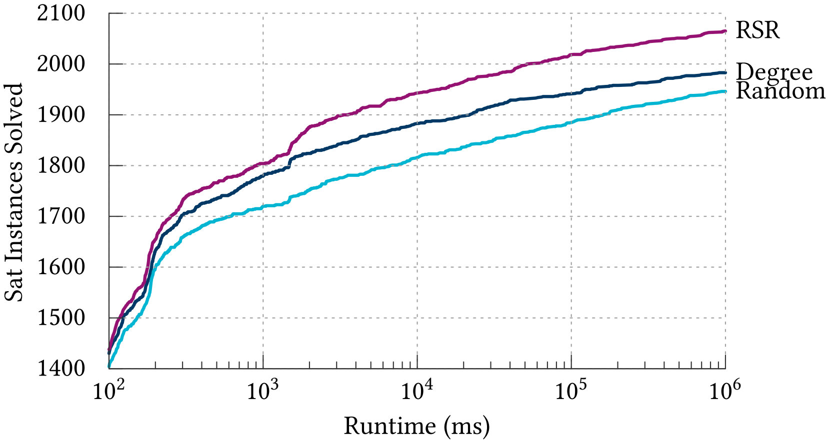


Random Search with Restarts and Nogood Recording

- Back to the random value-ordering heuristic.
- Aggressive restarts: every 100ms.
- Nogood recording and 2WL to avoid repeating work.

Random Search with Restarts and Nogood Recording



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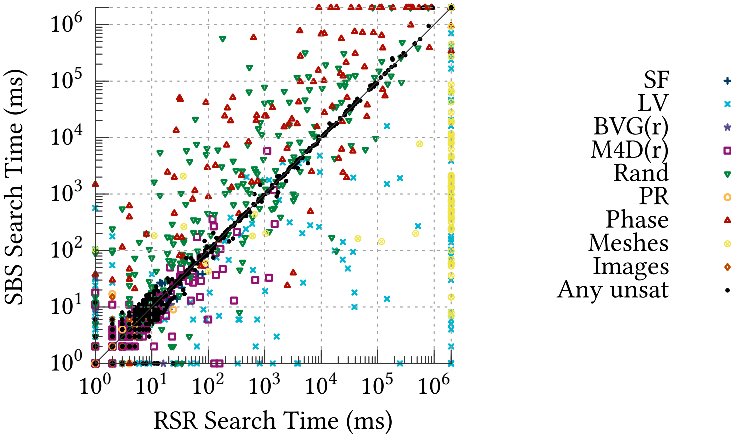


Value-Ordering Heuristics as Distributions

- Traditional view: value-ordering defines a search order.
- New view: value-ordering defines what proportion of the search effort should be spent on different subproblems.
- According to people who know more statistics than me, if solutions are uniformly distributed, then random search with restarts should be better than DFS.

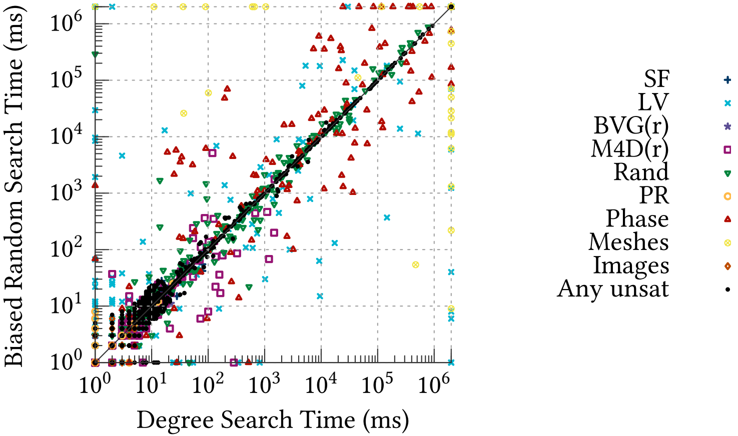
A Slightly Random Value-Ordering Heuristic

- For a fixed domain D_v, pick a vertex v' from a domain D_v with probability

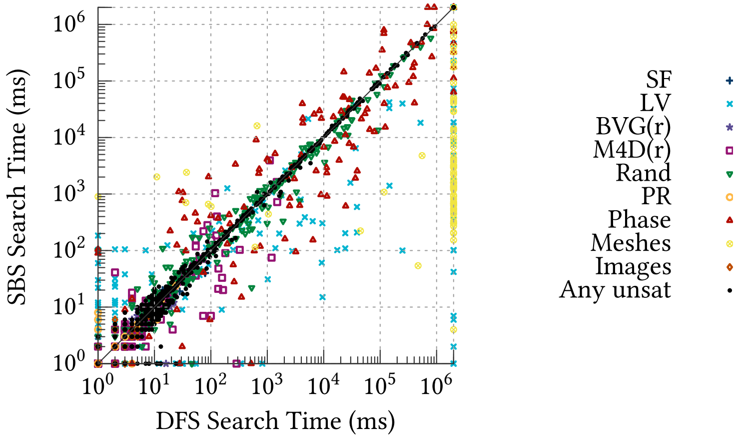
$$p(v') = \frac{2^{\deg(v')}}{\sum_{w \in D_v} 2^{\deg(w)}}$$

- Equally likely to pick between two vertices of degree d.
- Twice as likely to select a vertex of degree d than a vertex of degree $d - 1$.
- Justification: solution density and expected distribution of solutions.

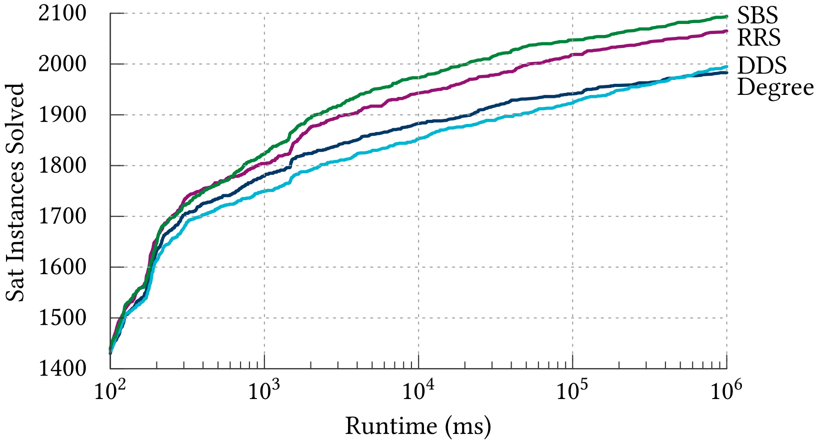
A Slightly Random Value-Ordering Heuristic



Is It Better?


SBS Search Time (ms)
DFS Search Time (ms)
10^0 10^1 10^2 10^3 10^4 10^5 10^6
SF
LV
BVG(r)
M4D(r)
Rand
PR
Phase
Meshes
Images
Any unsat

Is It Better?

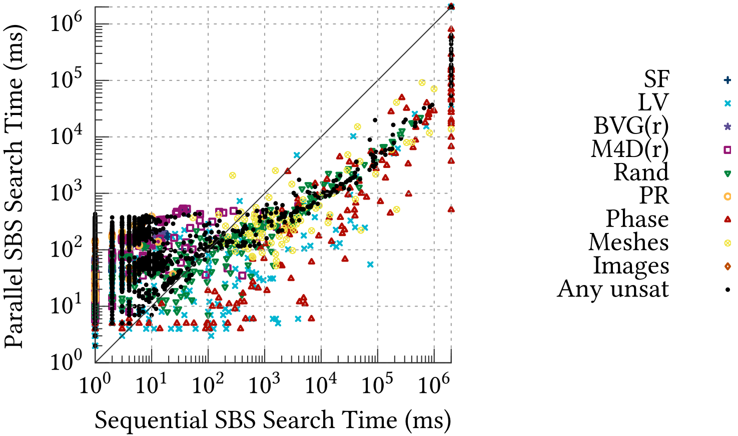


2100
2000
1900
1800
1700
1600
1500
1400
Sat Instances Solved
10^2
10^3
10^4
10^5
10^6
Runtime (ms)
SBS
RRS
DDS
Degree

Parallel Search

- Each thread gets its own random seed.
- Barrier synchronise on restarts.
- Share nogoods.

Is It Even Betterer?



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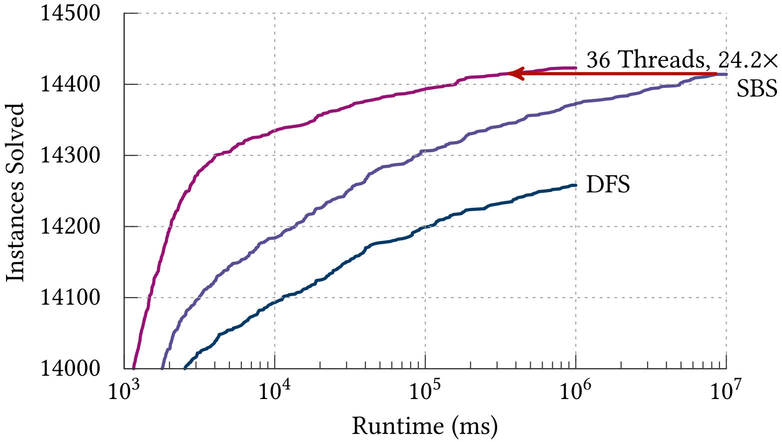

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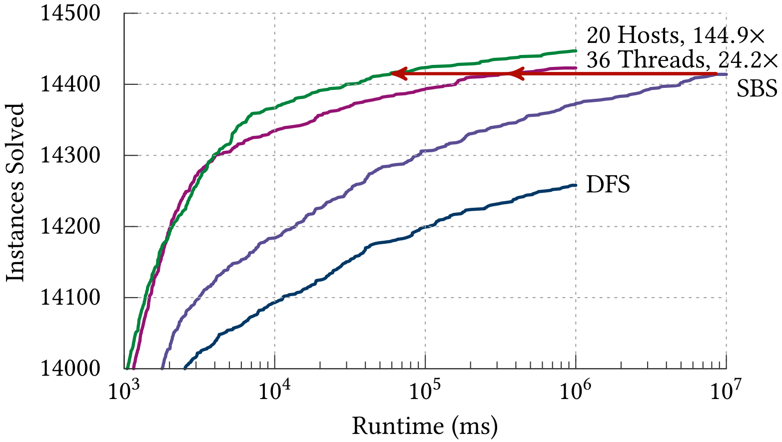
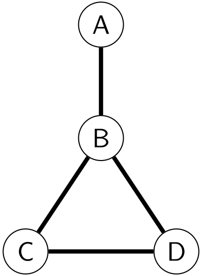


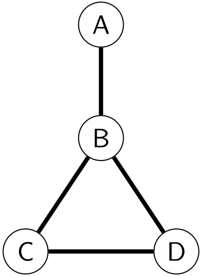
Lessons Learned

- Got to get a lot of things right:
  - Design.
  - Engineering.
  - Evaluation.
  - Understanding the hardware.
- Being clever only pays off if you can do it quickly.
  - Except sometimes it pays off even if it's really expensive.
- Not always clear what problem people really want to solve.

Symmetries

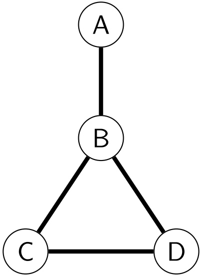


Symmetries



- Only find solutions where $C < D$.

Symmetries



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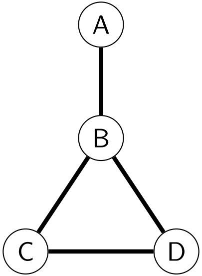
Symmetries



- Only find solutions where $C < D$.
- What about for arbitrary symmetries, in both pattern and target graphs?
- Dynamic symmetries?

Counting and Sampling

- We can easily enumerate all solutions.
- If we only need a count, can we speed things up?

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Counting and Sampling

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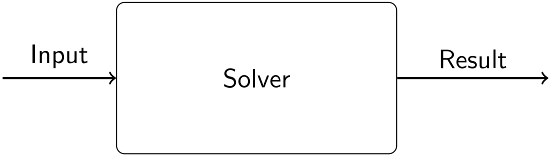
- What if an approximate count is OK?
- What if we want a few solutions, but sampled uniformly?
  - Common in term-rewriting systems.
- How does this interact with symmetries and decomposition?

Proof Logging



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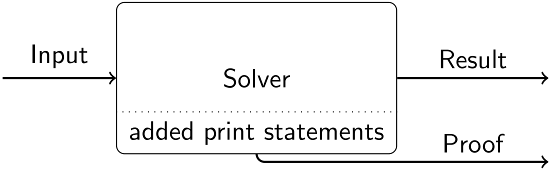

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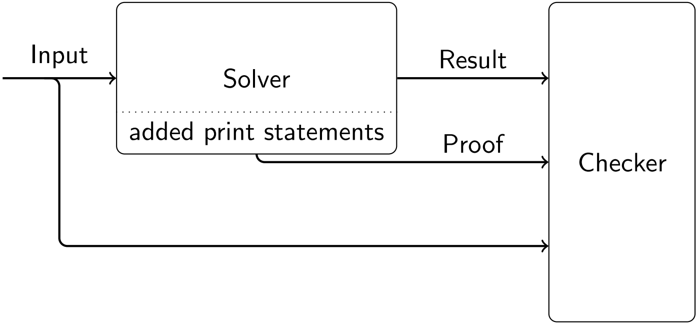

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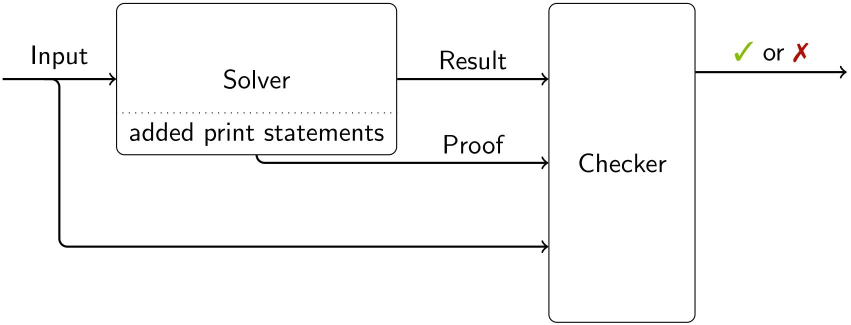

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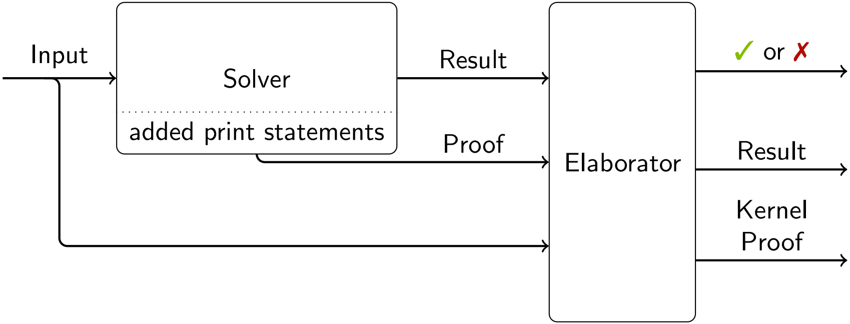

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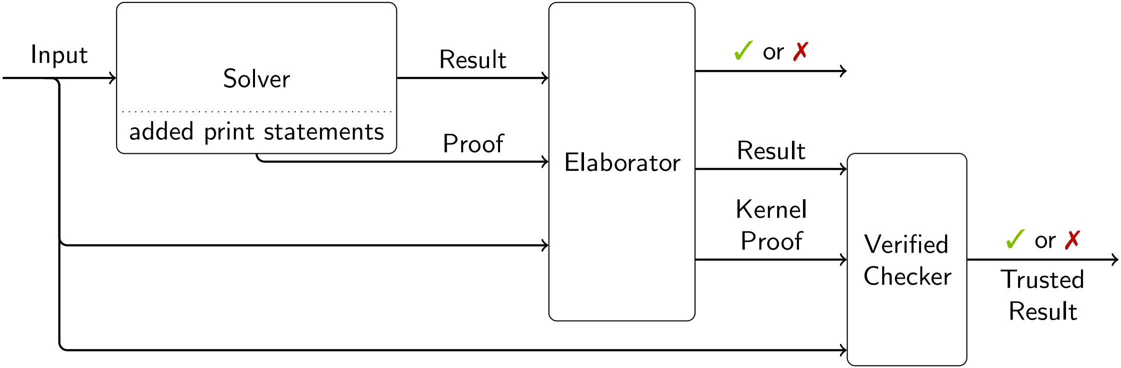

Components

- What if the target graph has two components?

Components

- What if the target graph has two components?
- What if the pattern graph has two components?

Components

- What if the target graph has two components?
- What if the pattern graph has two components?
- What if the graphs are "nearly" two components?

Learning

- Backtracking is bad. We should do CDCL!
- Except it doesn't seem to work very well...

Inference on Fancy Graphs

- What's the equivalent of neighbourhood degree sequence for directed graphs?
- What about if we have labels?
- Can these be computed efficiently?

Automatic Configuration

- What if the pattern graph is a triangle? A claw? One edge and one non-edge? A large clique?

Automatic Configuration

- What if the pattern graph is a triangle? A claw? One edge and one non-edge? A large clique?
- Which supplemental graphs should we use?
- Which inference rules are helpful?

Presolving

- Constraint programming solvers take too long to start up for “really easy” instances.
- Run a “fast” solver for 0.1s and then switch?

Presolving

- Constraint programming solvers take too long to start up for "really easy" instances.
- Run a "fast" solver for 0.1s and then switch?
- Doesn't help us for very solution-dense enumeration problems though.

Performance Portability

- Will algorithms designed on this year's hardware work well next year?

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- Or on Mac ARM hardware rather than Intel / AMD x64?

Performance Portability

- Will algorithms designed on this year's hardware work well next year?
- Or on Mac ARM hardware rather than Intel / AMD x64?
- On heterogeneous multi-core?

File Formats

- Design a graph file format that isn't terrible.

https://ciaranm.github.io/

ciaran.mccreesh@glasgow.ac.uk

University of Glasgow

Royal Academy of Engineering