# Finding Little Graphs Inside Big Graphs

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University of Glasgow

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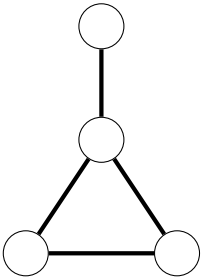
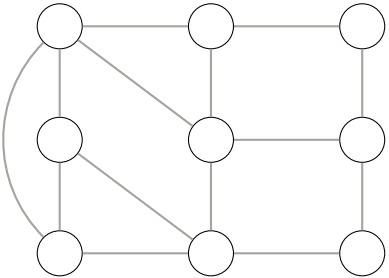
# Subgraph Isomorphism





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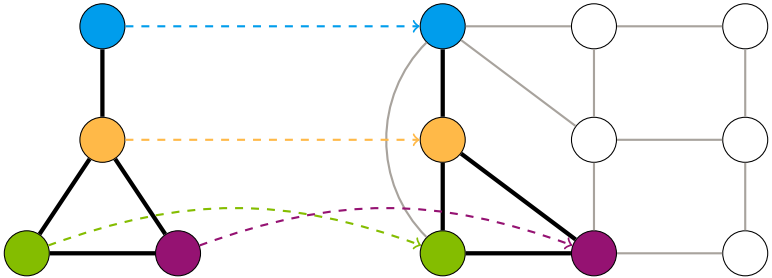

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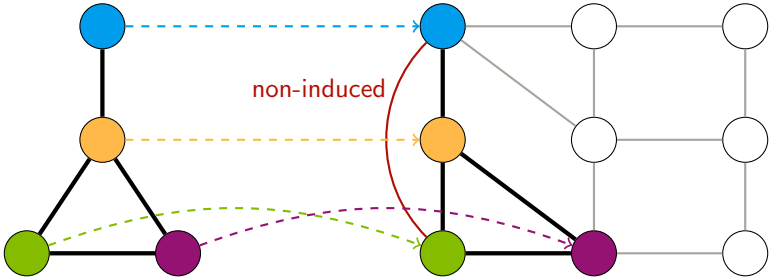

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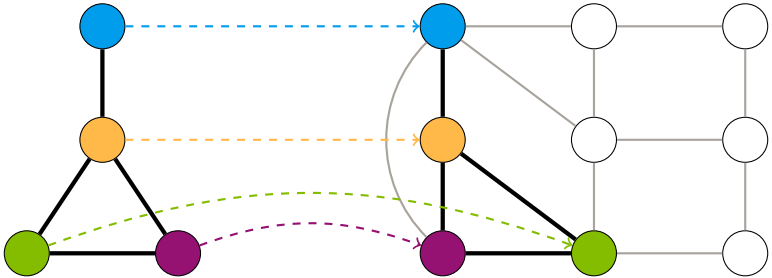

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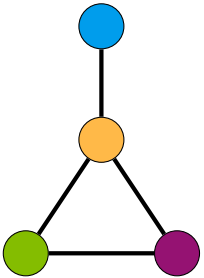

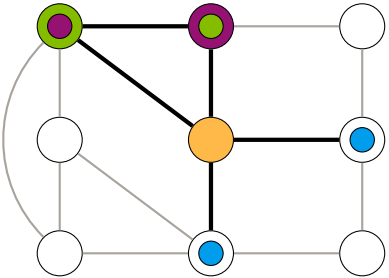

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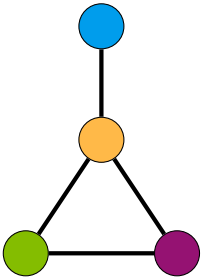

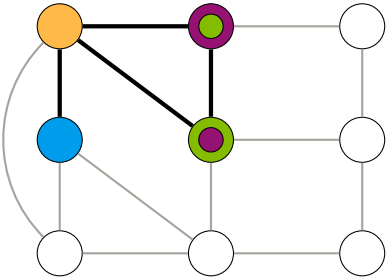

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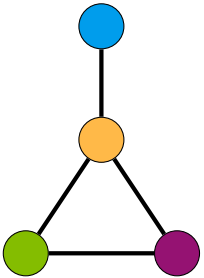

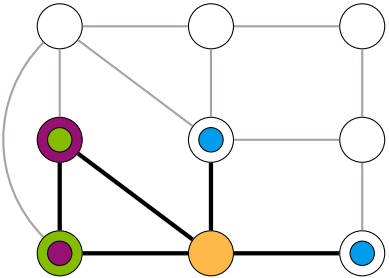

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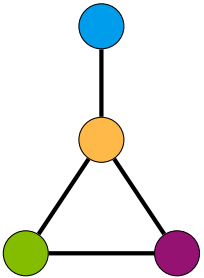

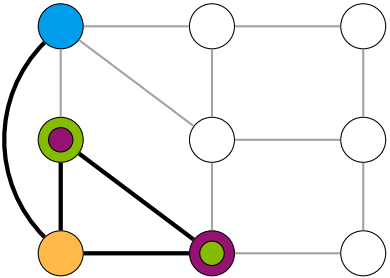

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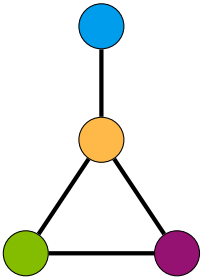

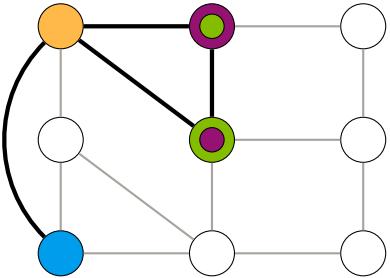

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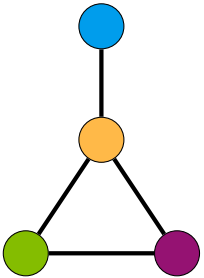
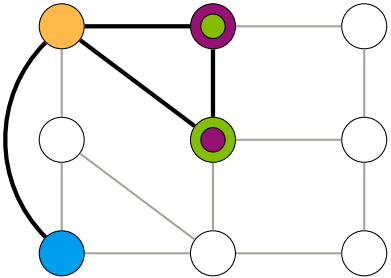
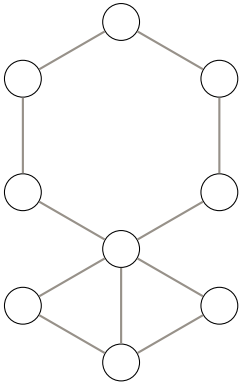
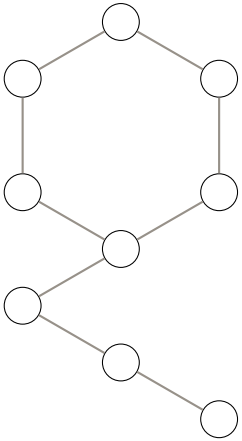




How many did I miss?

# Maximum Common Induced Subgraph





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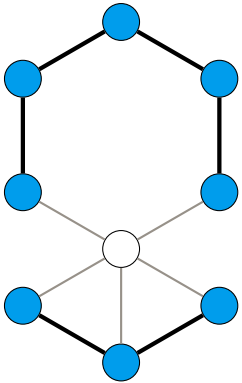
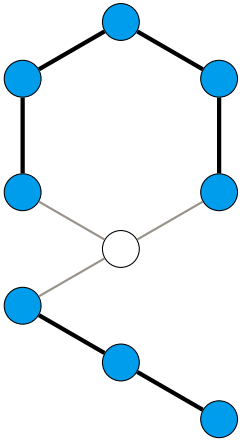
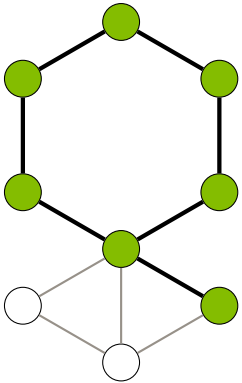
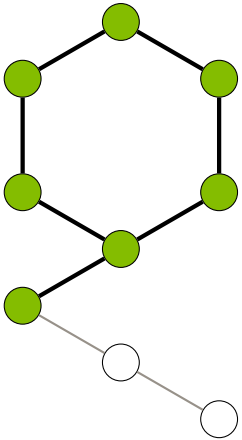




# Maximum Common Induced Connected Subgraph





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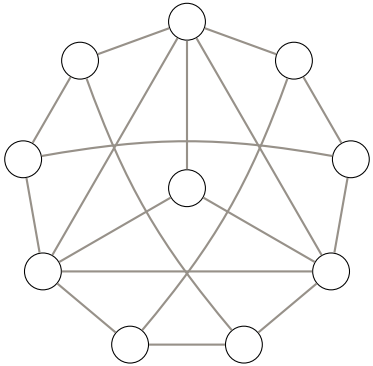

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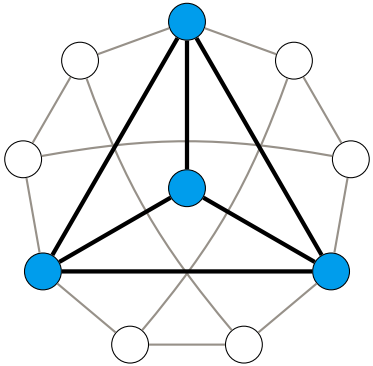

# Who Cares?

- 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.

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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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- No need for injectivity (homomorphism), or only local injectivity.
- 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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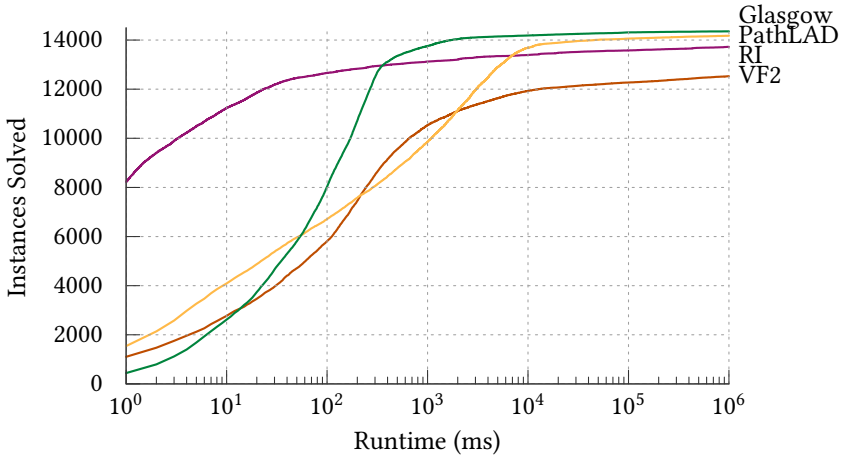
- Also special algorithms for clique.
- Guaranteed no bugs!
  - Or at least, any buggy output will always be detected, if you enable proof logging.

# 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.
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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.
- Must either be copyable, or have some way of doing backtracking.

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- We store a set of values for every variable.
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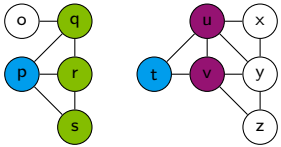
- Must either be copyable, or have some way of doing backtracking.
- Objectively correct answer: bitsets.

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

# Adjacency Filtering

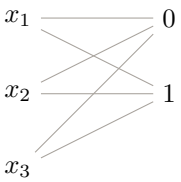
- When $P$ gets mapped to $t$, neighbours of $P$ can only be mapped to neighbours of $t$.
- Store domains and neighbourhoods as bitsets.

# 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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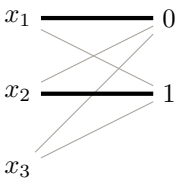

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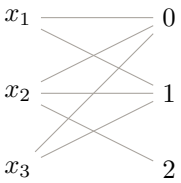

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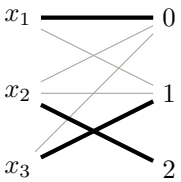
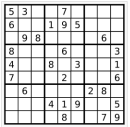


# Sudoku

From Wikipedia, the free encyclopedia

*Not to be confused with Sodoku or Sudeki.*

**Sudoku** (數独 *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.



A typical Sudoku puzzle

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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|---|---|---|---|---|---|---|---|---|
| 1 | 23 | 23 | 245 | 456 | 456 | 279 | 378 | 23589 |

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|---|---|---|---|---|---|---|---|---|
| 1 | 23 | 23 | 45 | 456 | 456 | 79 | 78 | 89 |

# Generalised Arc Consistency

- Generalised Arc Consistency (GAC): for a given 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

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|---|---|---|---|---|---|---|---|---|

$x_0$ 1

$x_1$ 2

$x_2$ 3

$x_3$ 4

$x_4$ 5

$x_5$ 6

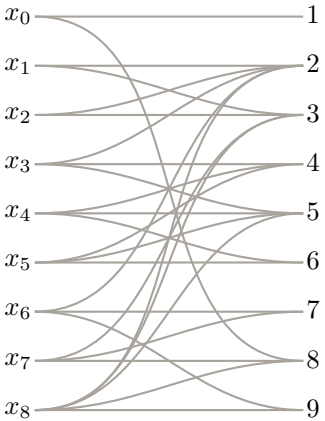
$x_6$ 7

$x_7$ 8

$x_8$ 9

# GAC for All-Different

| 18 | 23 | 23 | 245 | 456 | 456 | 279 | 378 | 23589 |
|---|---|---|---|---|---|---|---|---|



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| 18 | 23 | 23 | 245 | 456 | 456 | 279 | 378 | 23589 |
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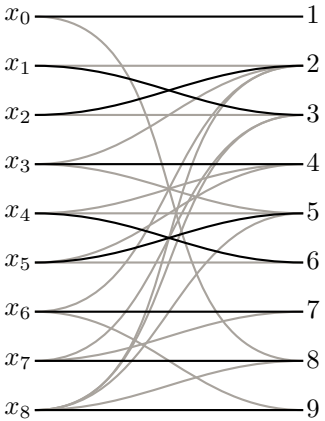

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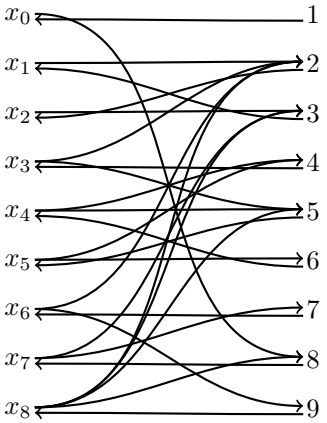

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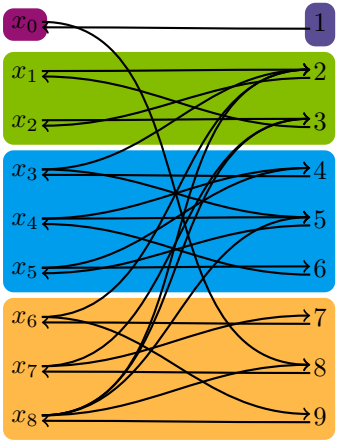

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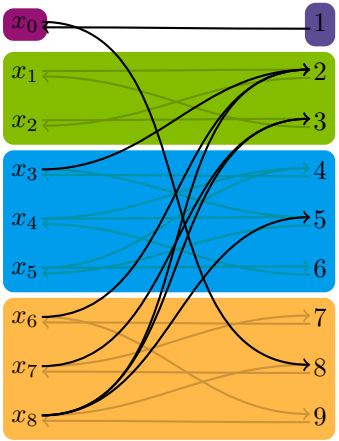

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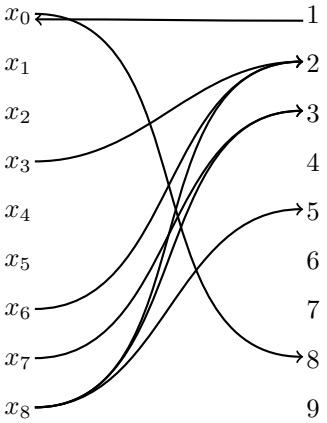

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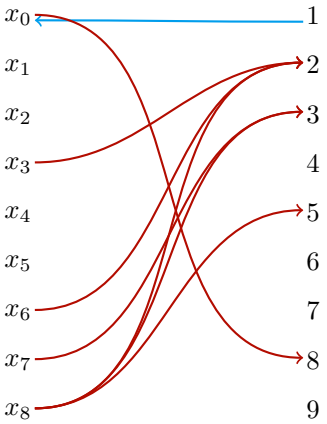

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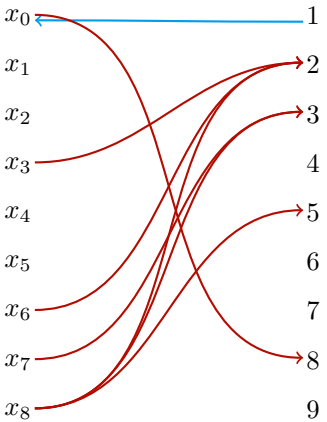


# Is This a Good Idea?

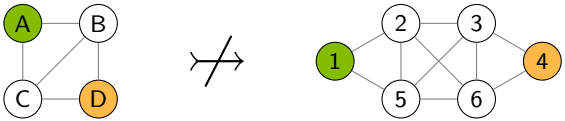
- Various techniques to avoid running all-different all of the time.
  - Faster bit-parallel propagator that can miss some deletions.
- Can also do all-different on edges...

# Distance Filtering

- Adjacent vertices must be mapped to adjacent vertices.

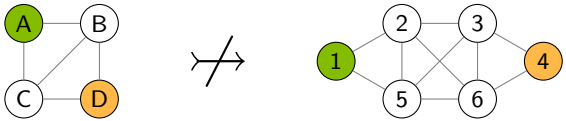
# Distance Filtering

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



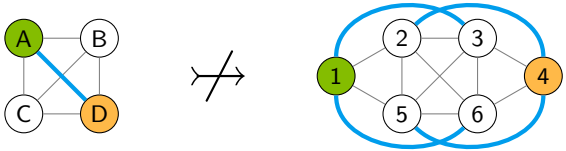
# Distance Filtering

- 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

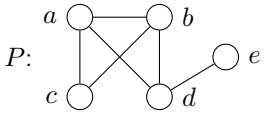
- $G^d$ is the graph with the same vertex set as $G$, and an edge between $v$ and $w$ if the distance between $v$ and $w$ in $G$ is at most $d$.
- For any $d$, a subgraph isomorphism $i : P \rightarrowtail T$ is also a subgraph isomorphism $i^d : P^d \rightarrowtail T^d$.

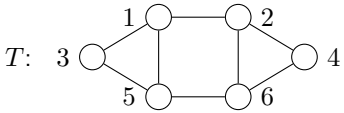


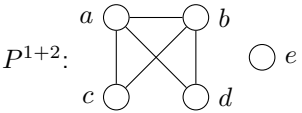
# Distance Filtering

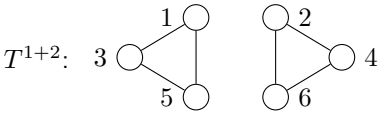
- We can do something stronger: rather than looking at distances, we can look at (simple) paths, and we can count how many there are.
- This is NP-hard in general, but only lengths 2 and 3 and counts of 2 and 3 are useful in practice.
- We construct these graph pairs once, at the top of search, and use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

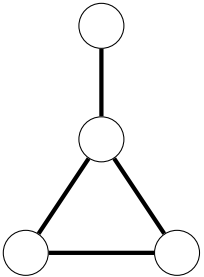
$$\overline{P} \rightarrowtail \overline{T}$$

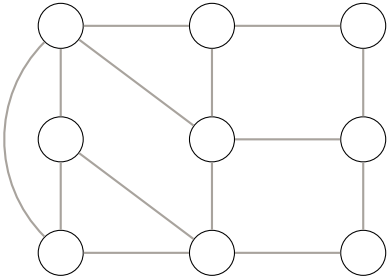
# Partially Defined Graphs

- 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).





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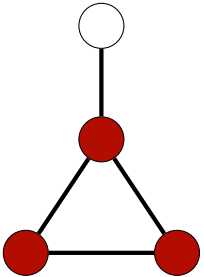
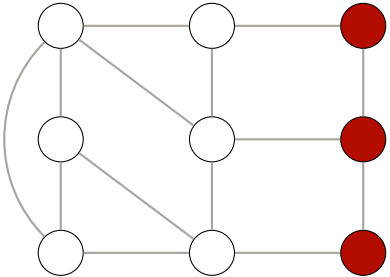
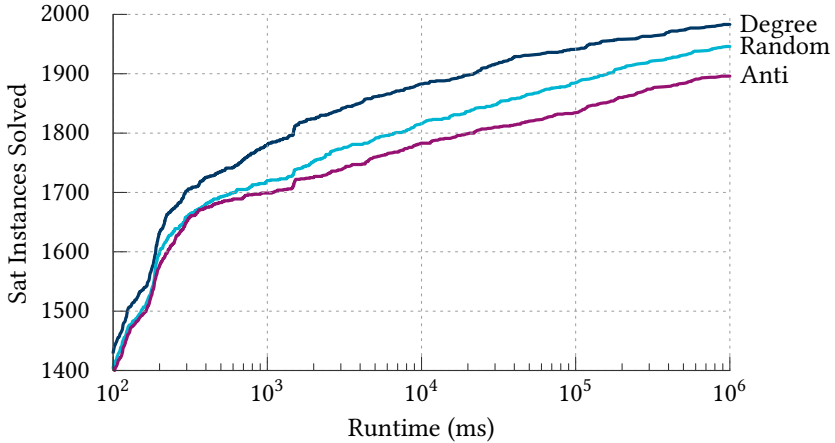




# Variable and Value Ordering Heuristics

- 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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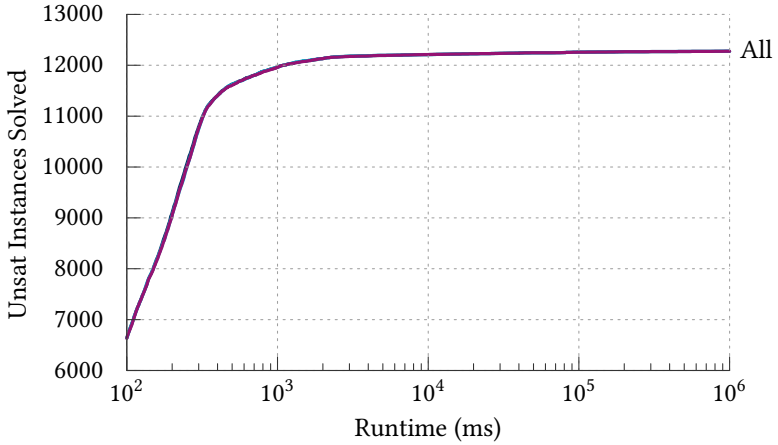
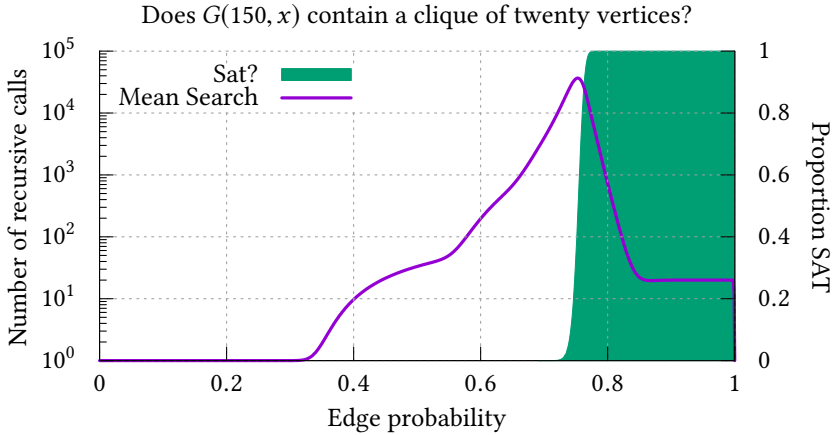


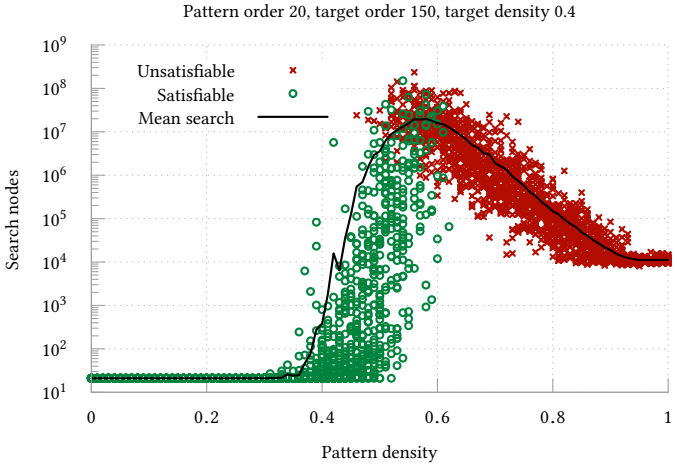
# Clique in Random Graphs



# 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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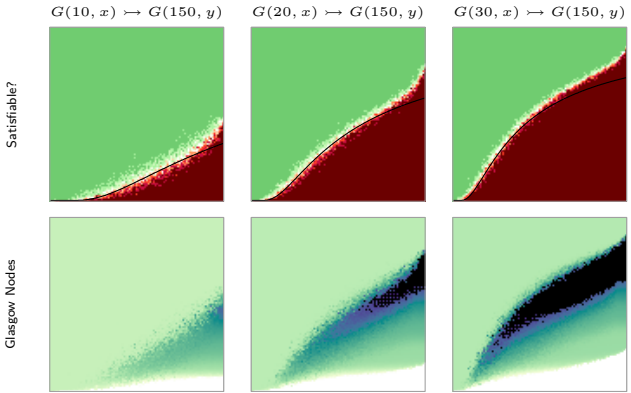

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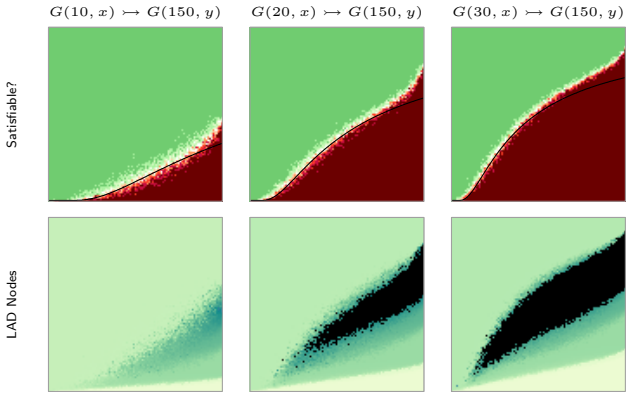

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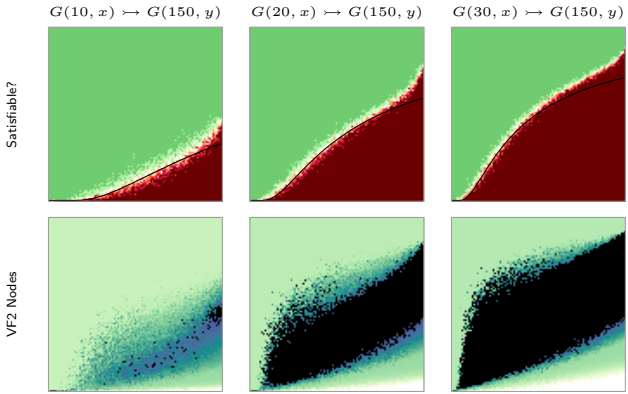


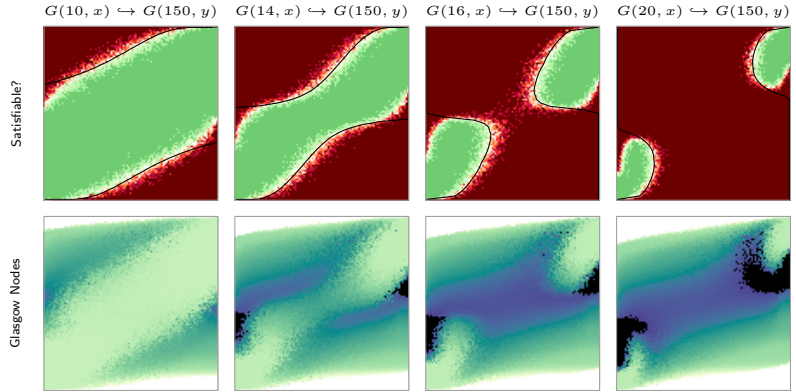
# Hand-Wavy Theoretical Justification

- 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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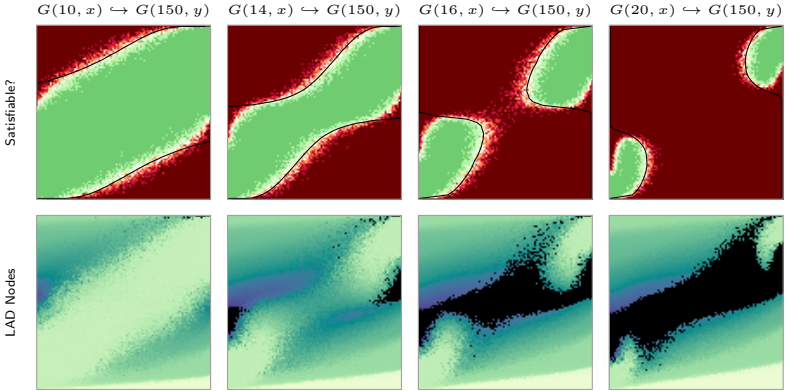

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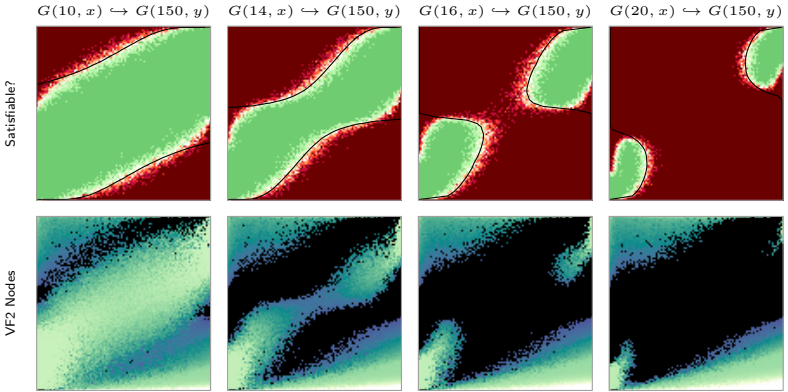

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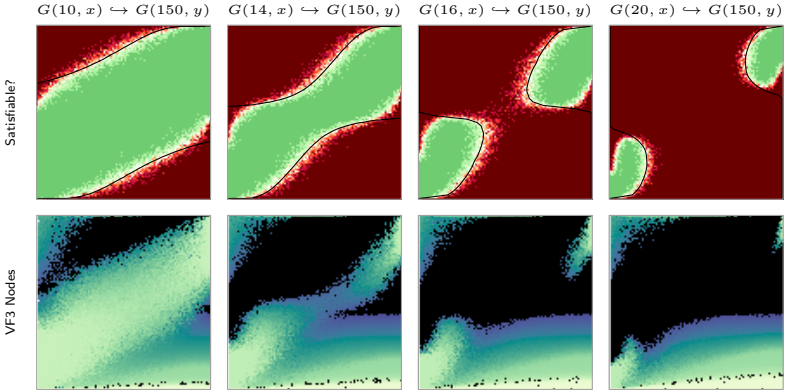
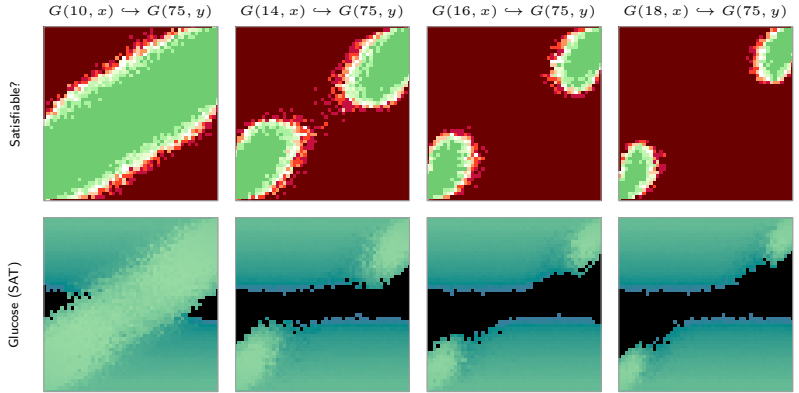


# Is This Algorithm-Independent?



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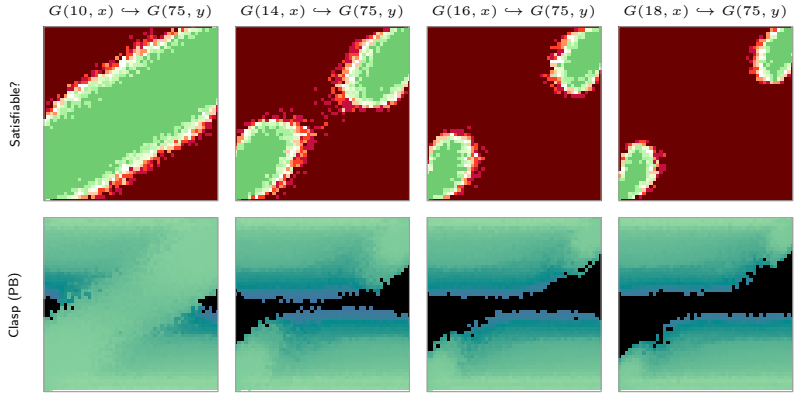

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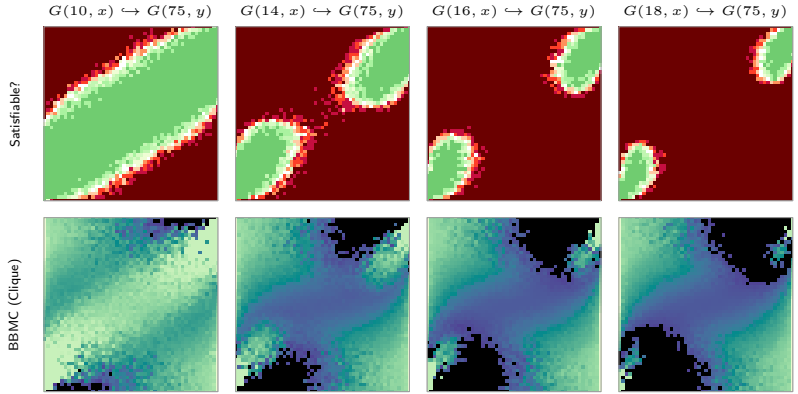

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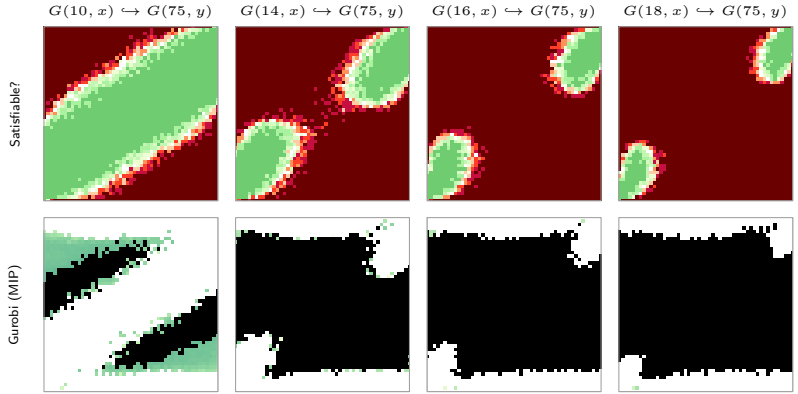
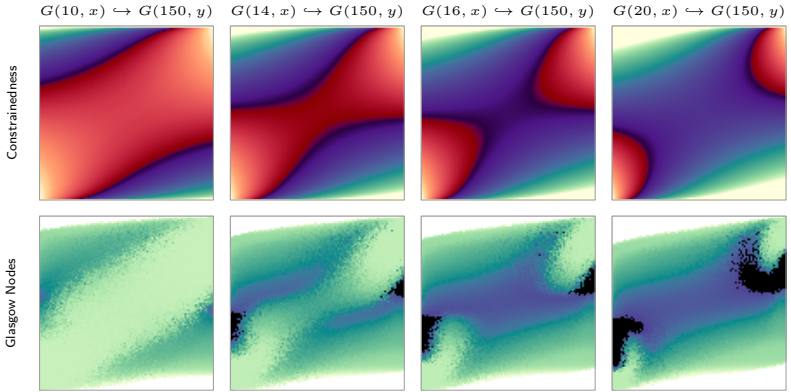


# Constrainedness

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

# Constrainedness

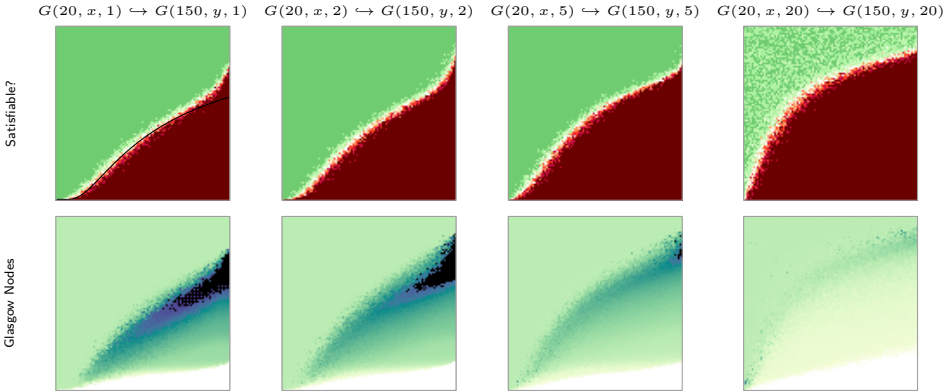


# Labelled Subgraph Isomorphism

- 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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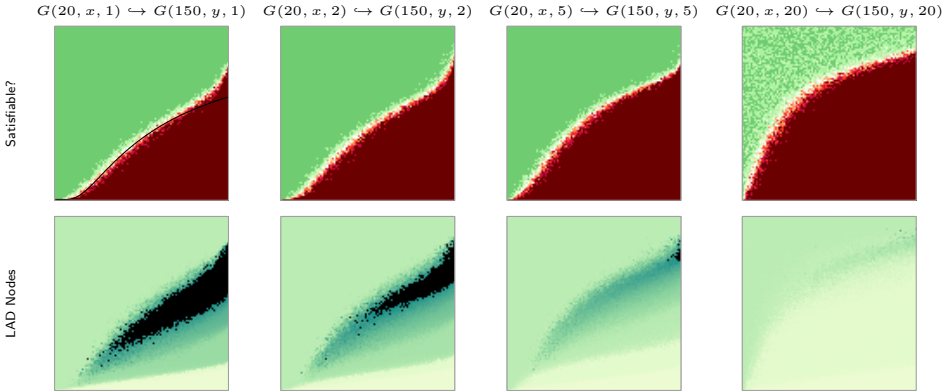

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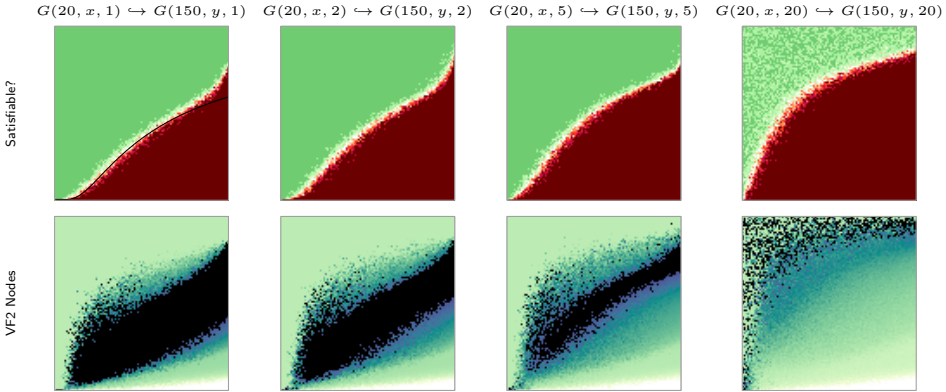
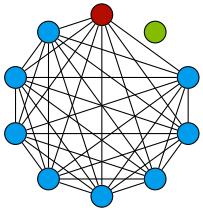
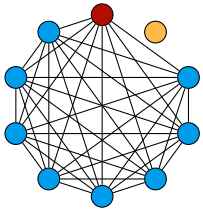


# Connectivity Algorithms are Really Stupid





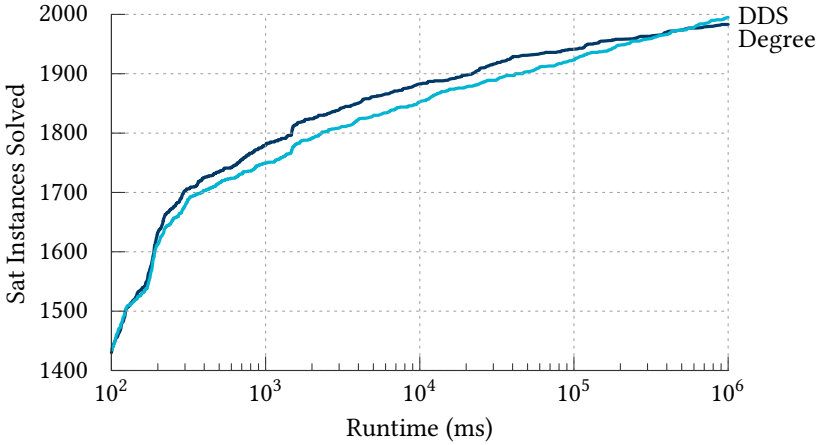
# Back to Value-Ordering Heuristics

- Largest target degree first.

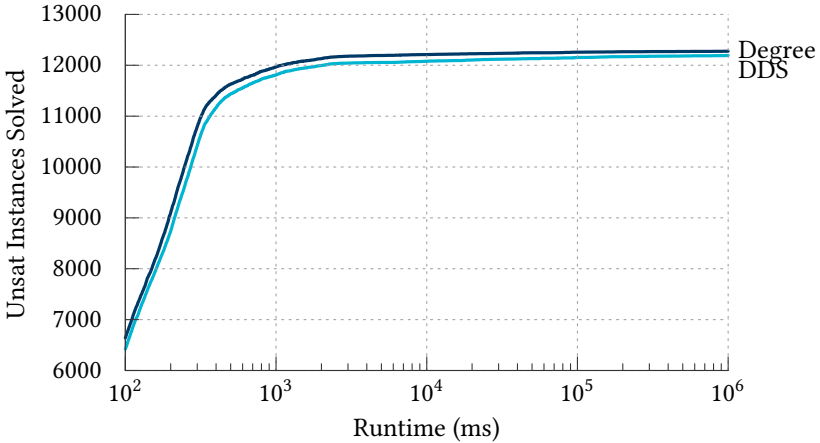
# However. . .

- 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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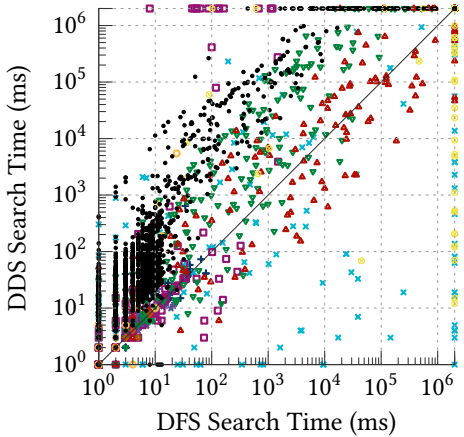
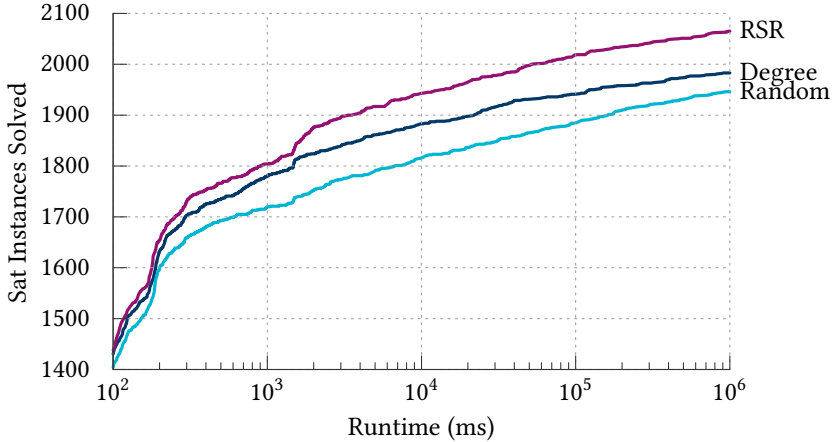


# Random Search with Restarts and Nogood Recording

- 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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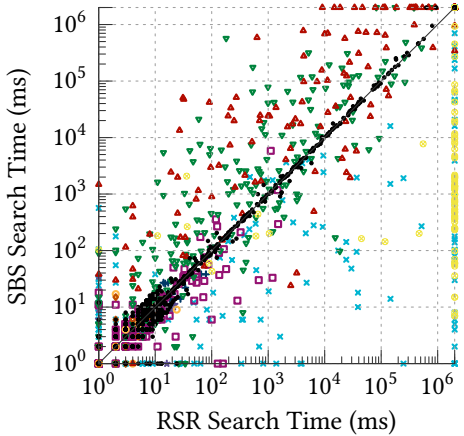


# Value-Ordering Heuristics as Distributions

- 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.

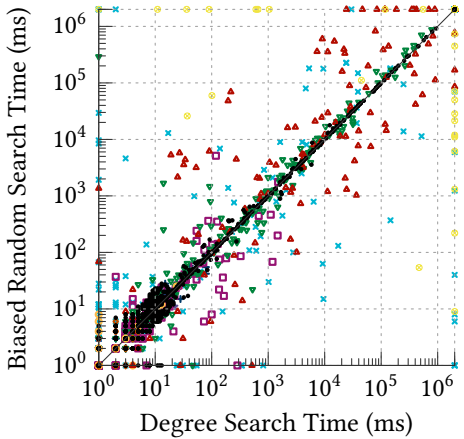
# A Slightly Random Value-Ordering Heuristic

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

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

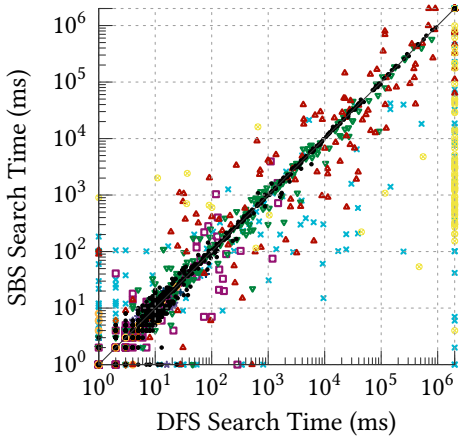
- Equally likely to pick between two vertices of degree $d$.
- Twice as likely to select a vertex of degree $d$ than a vertex of degree $d - 1$.
- Justification: solution density and expected distribution of solutions.

# A Slightly Random Value-Ordering Heuristic




SF
LV
BVG(r)
M4D(r)
Rand
PR
Phase
Meshes
Images
Any unsat

# 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

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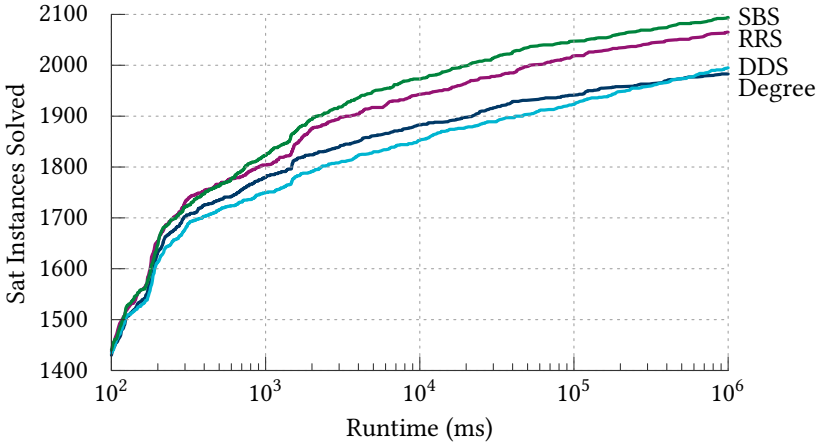
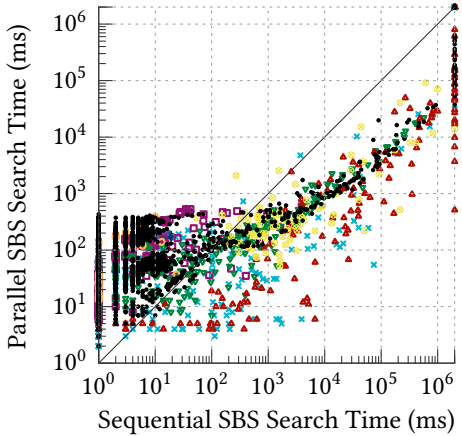

2100
2000
1900
1800
1700
1600
1500
1400
Sat Instances Solved
$10^2$
$10^3$
$10^4$
$10^5$
$10^6$
Runtime (ms)
SBS
RRS
DDS
Degree

# Parallel Search

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

# Is It Even Betterer?

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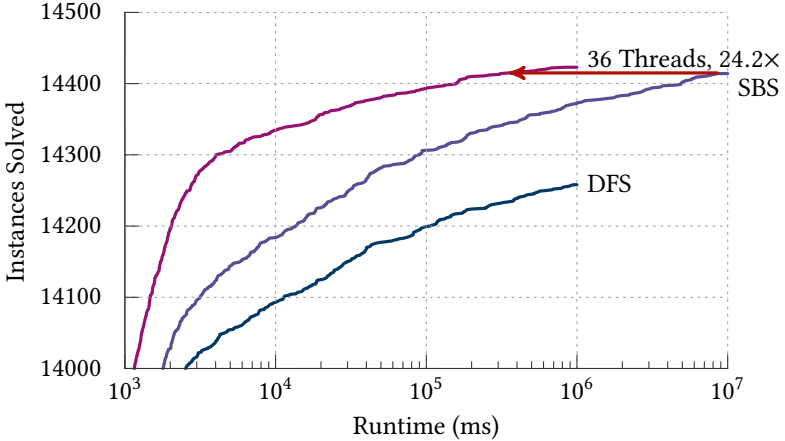

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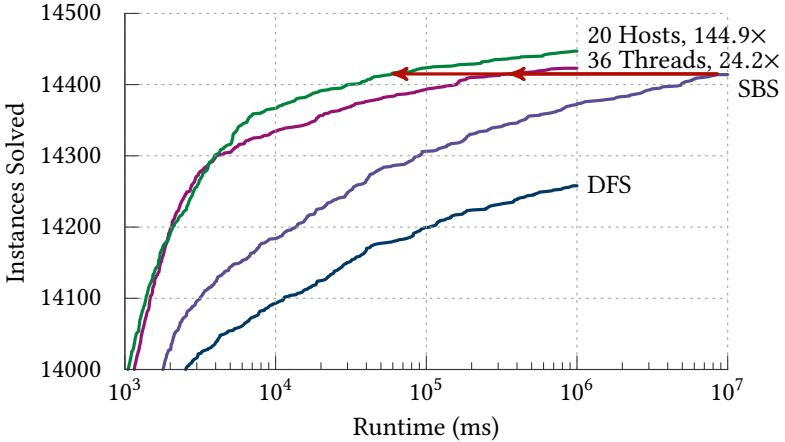
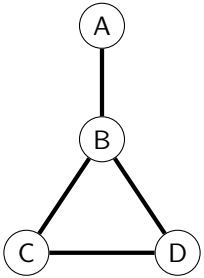


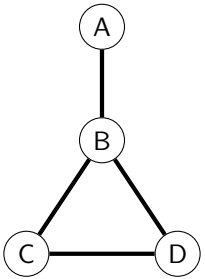
# Lessons Learned

- 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

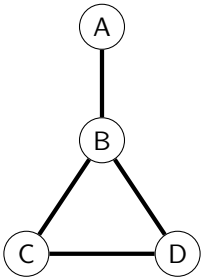


# Symmetries




- Only find solutions where $C < D$.

# Symmetries

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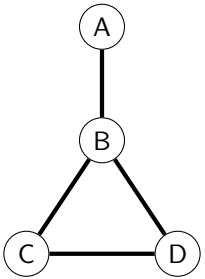


- Only find solutions where $C < D$.
- What about for arbitrary symmetries, in both pattern and target graphs?
- Dynamic symmetries?

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- What if an approximate count is OK?
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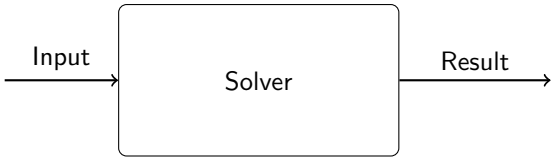
  - Common in term-rewriting systems.
- How does this interact with symmetries and decomposition?

# Proof Logging



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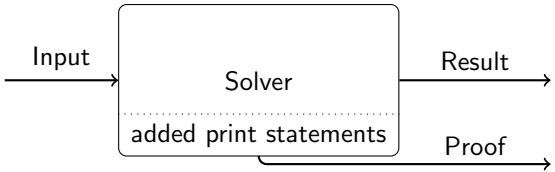

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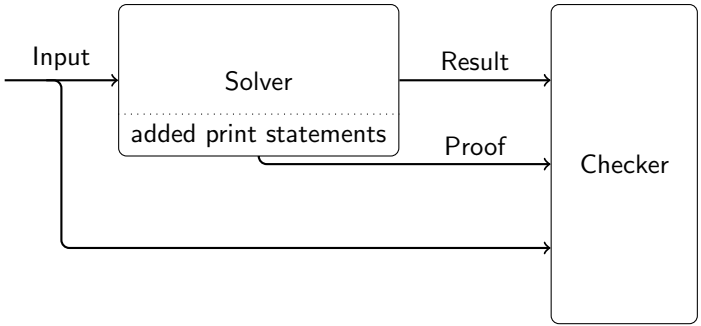

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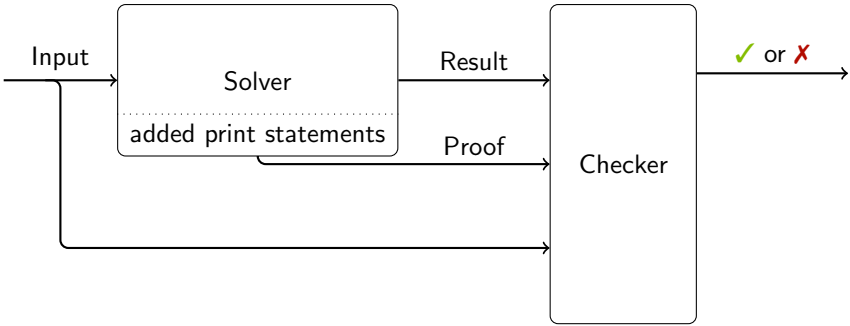

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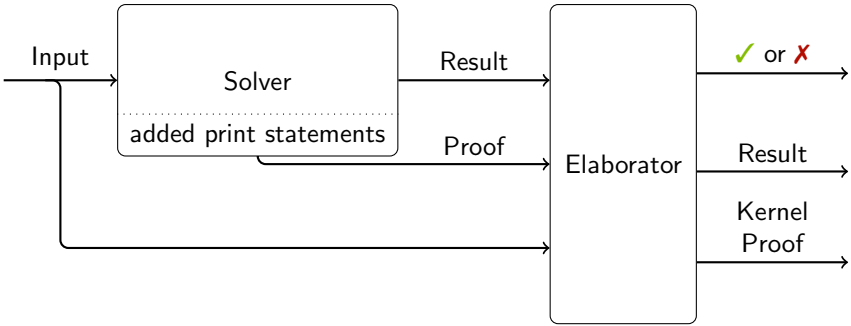

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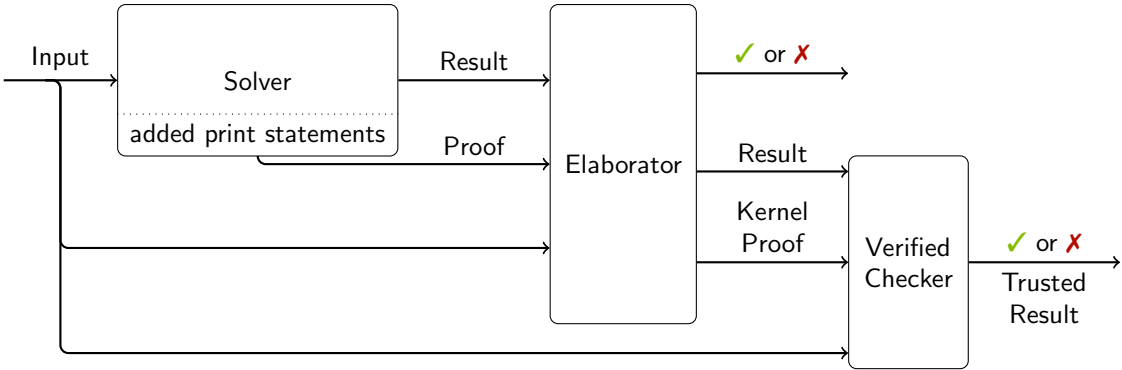

# Components

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- 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?

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- 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.

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- 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/

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University of Glasgow

Royal Academy of Engineering