Finding Little Graphs Inside Big Graphs (in Parallel)

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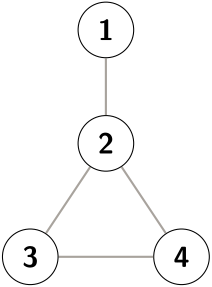
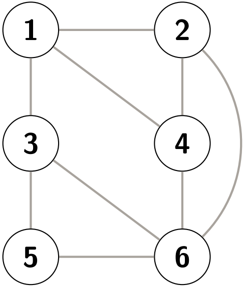
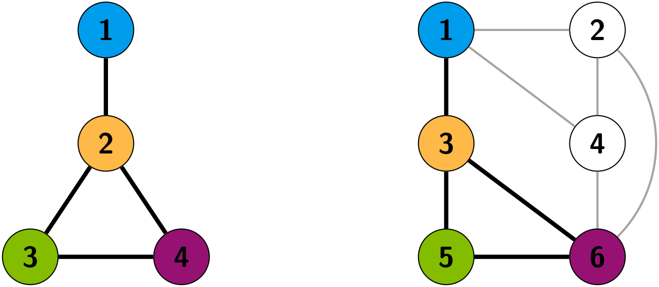
Subgraph Isomorphism





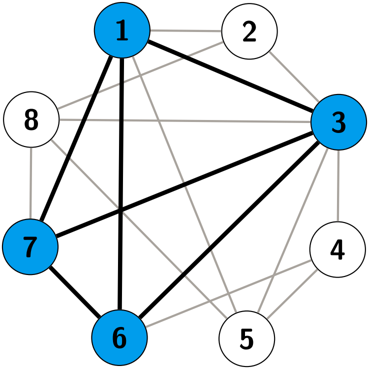
Subgraph Isomorphism



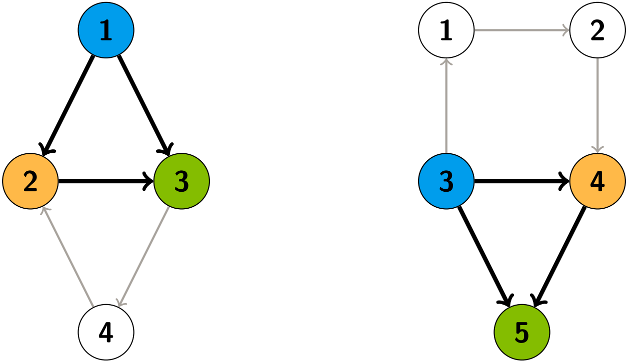
Subgraph Isomorphism

- Find an *injective* mapping from a *pattern* graph to a *target* graph.
- **Adjacent** vertices must be **mapped to adjacent** vertices.
- For the *induced* problem variant, non-adjacent vertices must be mapped to non-adjacent vertices.

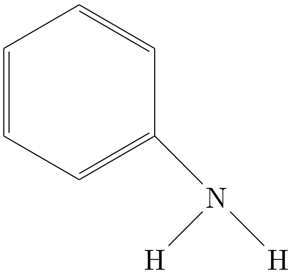
The Maximum Clique Problem

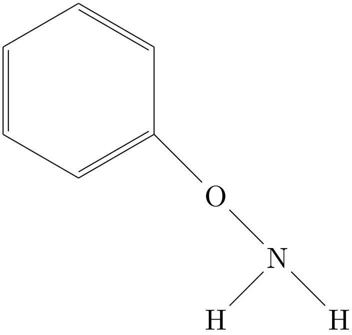


Maximum Common Subgraph



Maximum Common Connected Subgraph?





Who Cares?

- Bioinformatics
- Chemistry
- Drug design
- Computer vision
- Pattern recognition
- Financial fraud detection
- Model checking
- Fault detection
- Law enforcement
- Kidney exchange
- Social network analysis
- Compilers
- Diseased cows
- Computer algebra
- Circuit design
- Network design

Practical Algorithms

- Real-world inputs rarely have nice properties (low treewidth, particular degree spreads that are polynomial, etc).
- We can still solve some subgraph isomorphism problems with **thousand vertex patterns** and **ten thousand vertex targets** in a few seconds.
- Worst-case analysis is useless, and constant factors matter.

Constraint Models

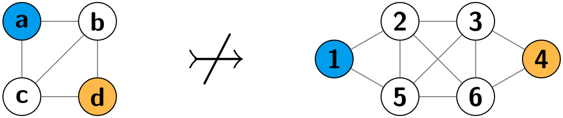
- We have some **variables**, each with a **domain**, and we want to give each variable a value from its domain.
  - Subgraph isomorphism: a variable for each pattern vertex, with domains being target vertices.
  - Clique: a boolean variable for each vertex.
- There are **constraints** between variables.
  - Subgraph isomorphism: all-different (injectivity), and adjacent pairs of vertices must be mapped to adjacent pairs of vertices.
  - Clique: for each pair of non-adjacent vertices, at least one of the two variables must be false.
- There is an **objective**.
  - Subgraph isomorphism: give each variable a value.
  - Maximum clique: set as many variables to true as possible.

Inference

- We want to **cross out values** from domains, until only one value is left in each.
- Subgraph isomorphism: high degree vertices cannot be mapped to low degree vertices.
- If an assignment becomes forced, we can **infer additional deletions**. This can have a cascade effect.

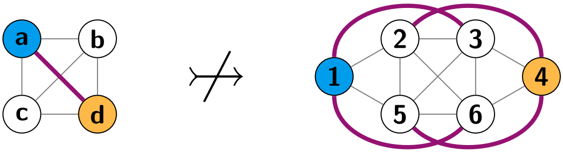
Implied Constraints for Subgraph Isomorphism

- 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.



Implied Constraints for Subgraph Isomorphism

- 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 $i^d : P^d \rightarrowtail T^d$.



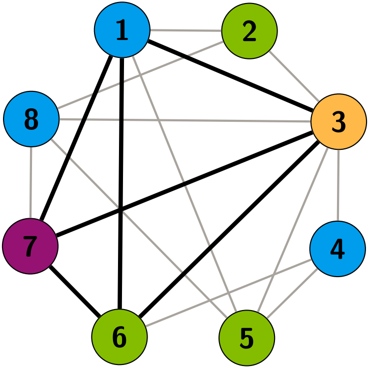
Implied Constraints for Subgraph Isomorphism

- 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.
- We can also use these graph pairs for degree-based filtering.

Search

- Sometimes we have to **guess**: pick a variable x. Then for each value v_i in its domain in turn, see what happens if we force $x = v_i$.
- There are good heuristics telling us which variable to pick first.
- There are heuristics telling us which value to pick first, but this seems to be less reliable in general.

Branch and Bound

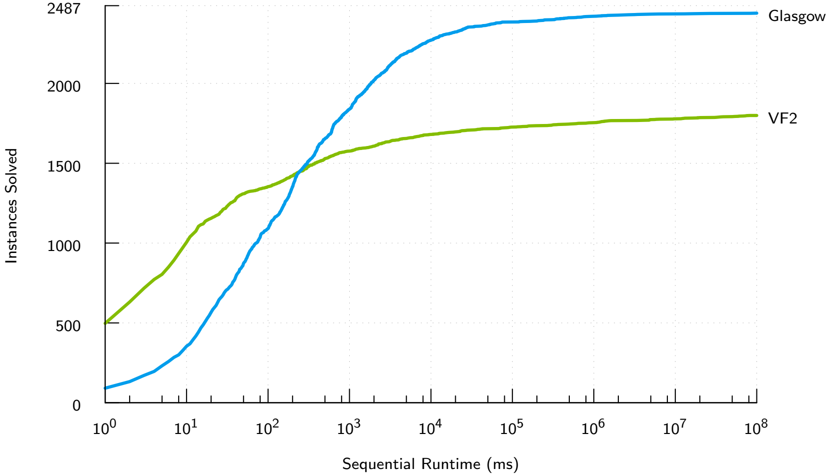


- For optimisation: keep track of the **best solution** we've found so far. If we can show we can't beat it, backtrack immediately.

Backjumping

- When backtracking, see if the current assignment actually removed any values which could have helped prevent the failure. If not, **jump back** another step.

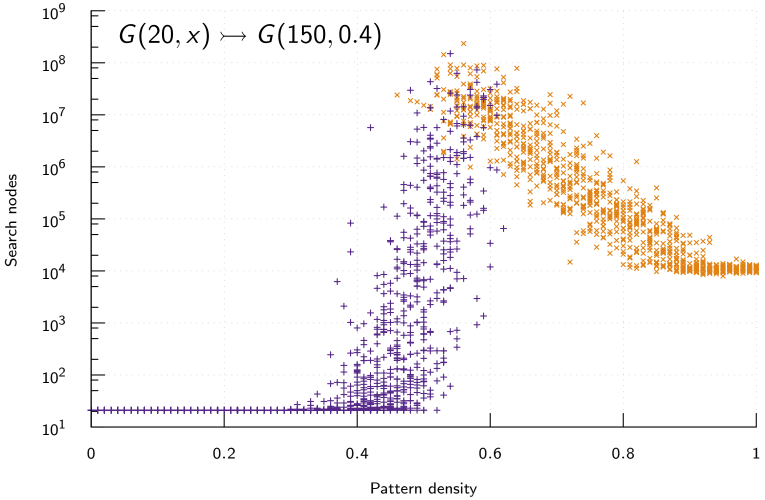
Is This Any Good?



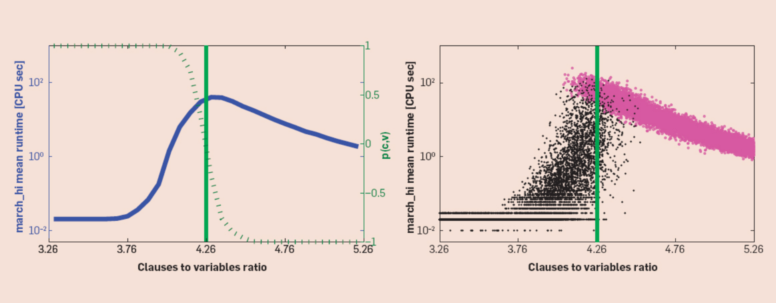
Generating Hard Subgraph Isomorphism Instances

- We can solve some problem instances with a thousand pattern vertices, and ten thousand target vertices. Can we solve *any* instance with these sizes?
- We like having **lots of instances**, to make sure we don't overfit algorithm parameters.
- How do we create random subgraph isomorphism instances?

Phase Transitions in Non-Induced Subgraph Isomorphism

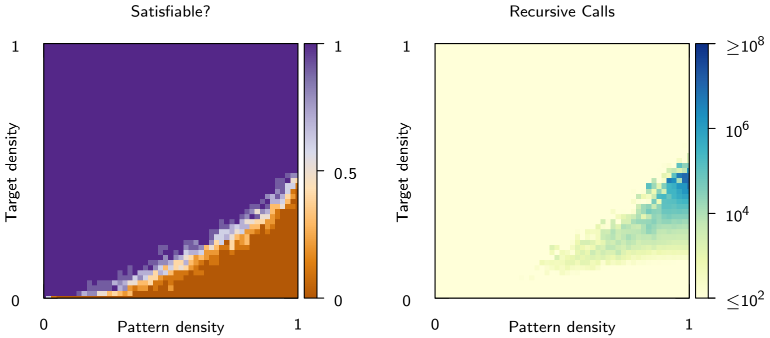


This Looks Familiar. . .



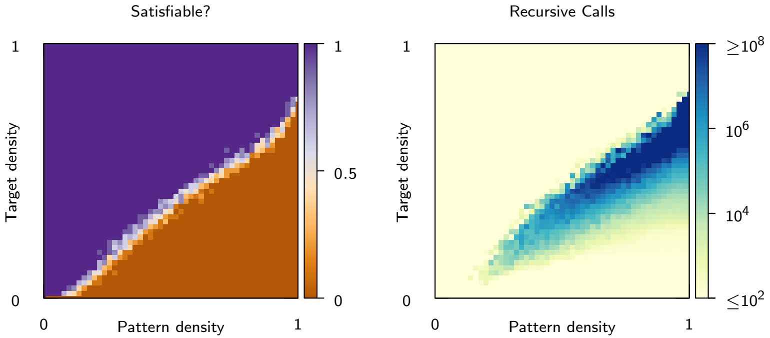
Understanding the Empirical Hardness of NP-Complete Problems.
Kevin Leyton-Brown, Holger H. Hoos, Frank Hutter, Lin Xu.
Communications of the ACM, Vol. 57 No. 5, Pages 98-107

Varying Both Densities?



$$G(10, x) \rightarrowtail G(150, y)$$

Varying Both Densities?



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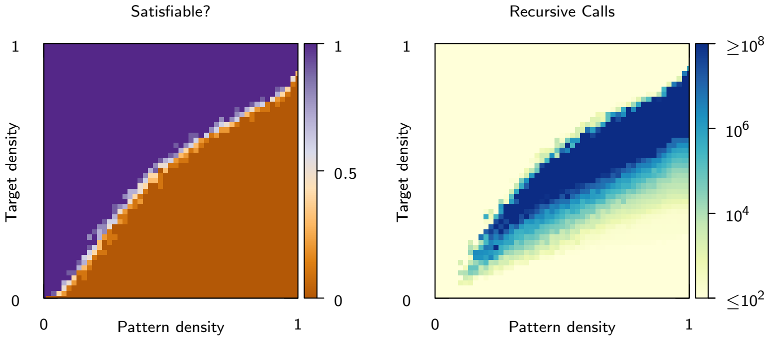


$$G(30, x) \rightarrowtail G(150, y)$$

Heuristics from Maximising Expectations

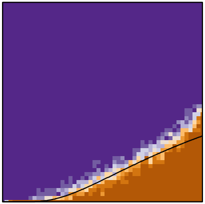
- With a few dubious assumptions regarding independence and integers, the expected number of solutions is

$$\langle Sol \rangle = t \cdot (t-1) \cdot \ldots \cdot (t-p+1) \cdot {d_t}^{d_p \cdot \binom{p}{2}}.$$

- If $\langle Sol \rangle \ll 1$, the instance is likely to be unsatisfiable.
- Unfortunately, if $\langle Sol \rangle \gg 1$, things are a bit trickier...

Heuristics from Maximising Expectations

$G(10, x) \rightarrowtail G(150, y)$



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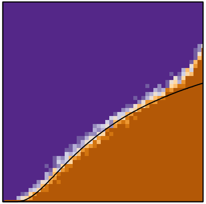

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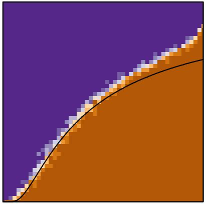


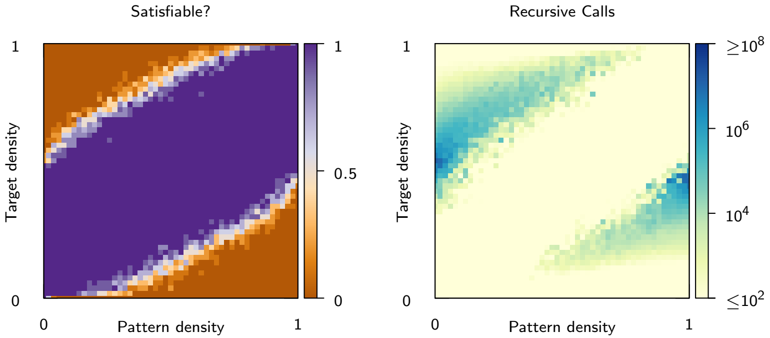
Heuristics from Maximising Expectations

- Suppose we wanted to maximise the expected number of solutions in a subproblem during search.

$$\langle Sol \rangle = \underbrace{t \cdot (t-1) \cdot \ldots \cdot (t-p+1)}_{\text{smallest domain}} \cdot \underbrace{d_t}_{\substack{\text{low}\\ \text{degree}}} {}^{\underbrace{d_p \cdot \binom{p}{2}}_{\substack{\text{high}\\ \text{degree}}}}$$

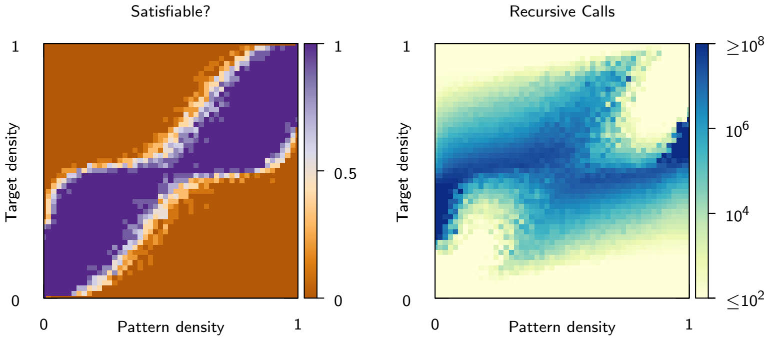
- These heuristics are used in practice (sort of), but were discovered through guessing and experiments!

Phase Transitions in Induced Subgraph Isomorphism



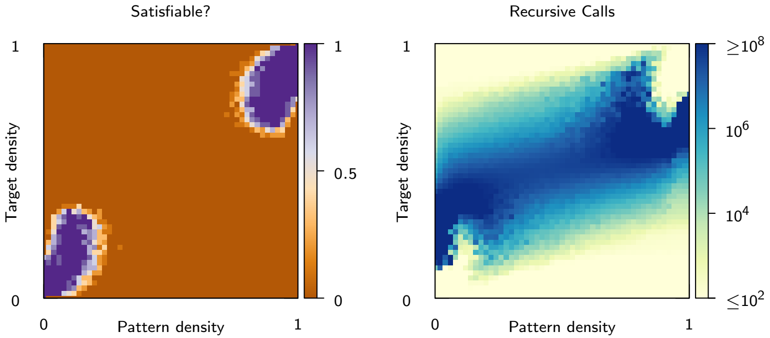
$$G(10, x) \hookrightarrow G(150, y)$$

Phase Transitions in Induced Subgraph Isomorphism



$$G(15, x) \hookrightarrow G(150, y)$$

Phase Transitions in Induced Subgraph Isomorphism



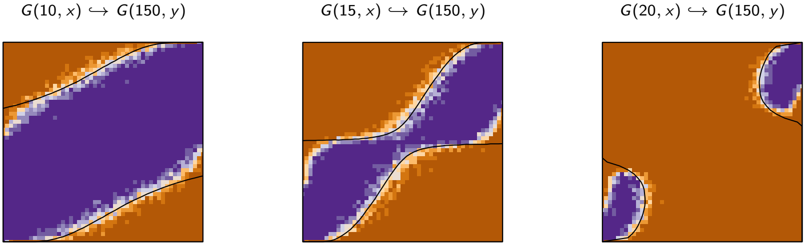
$$G(20, x) \hookrightarrow G(150, y)$$

Can We Predict This?

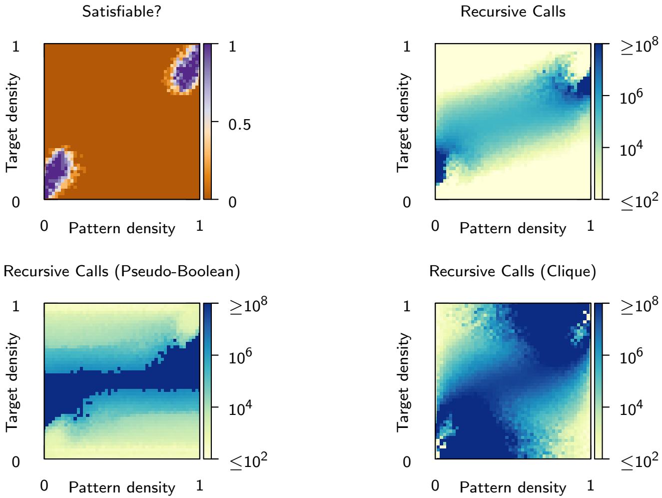
- With a few more dubious assumptions, the expected number of solutions is now

$$\langle Sol \rangle = t \cdot (t-1) \cdot \ldots \cdot (t-p+1) \cdot {d_t}^{d_p \cdot \binom{p}{2}} \cdot (1-d_t)^{(1-d_p) \cdot \binom{p}{2}}.$$

Can We Predict This?



Why is the Middle Region Hard?



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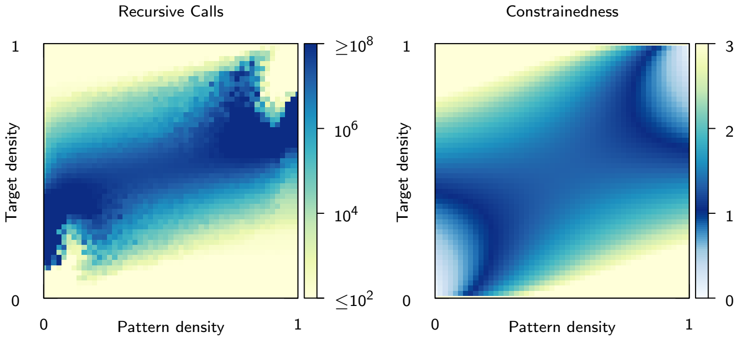
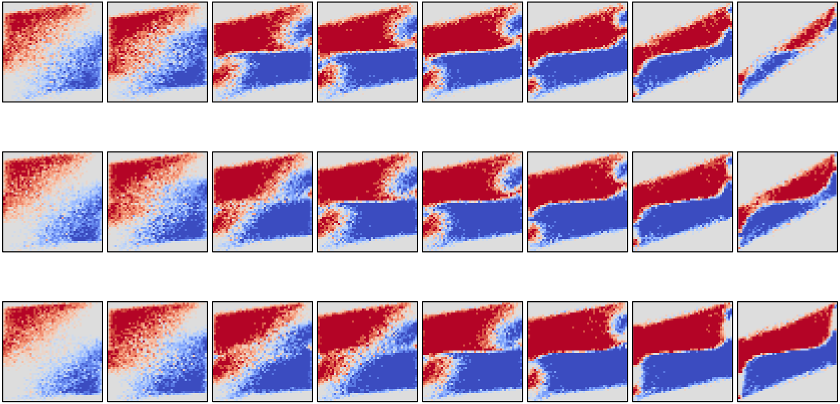


$$G(20, x) \hookrightarrow G(150, y)$$

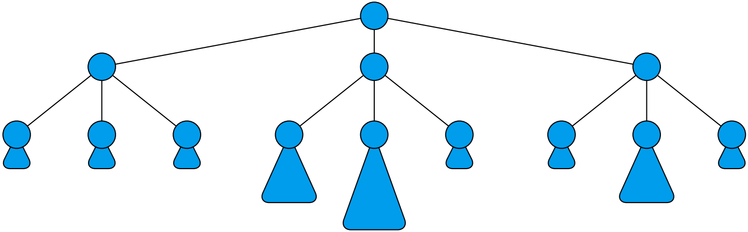
Induced Heuristics?

- For anything we say about degree, the opposite holds for the complement constraints.
- Degree-based value ordering heuristics don't seem to help. This is intuitive, but does this formula give us a heuristic after all?

Induced Heuristics?



Thread-Parallel Tree Search



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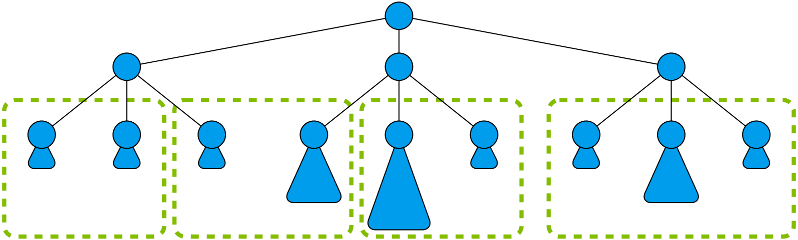

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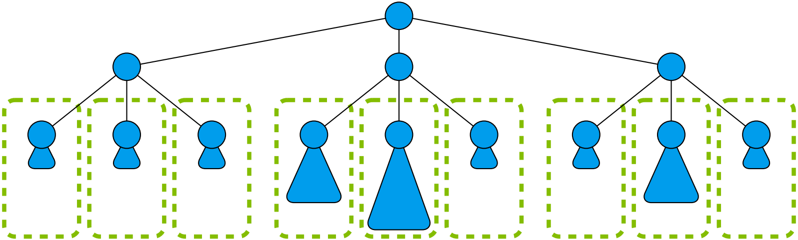
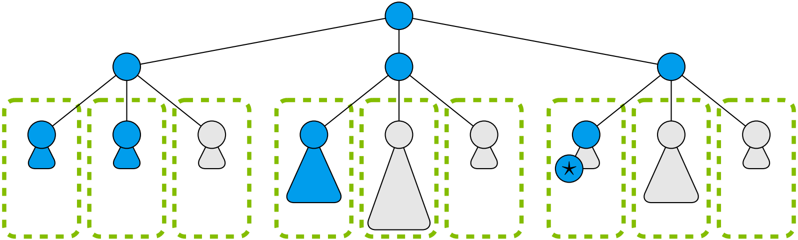


Parallel Search Order Matters



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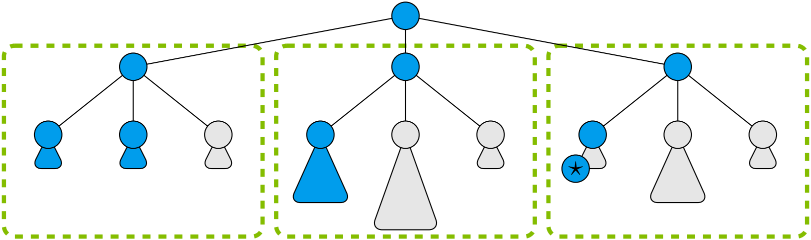

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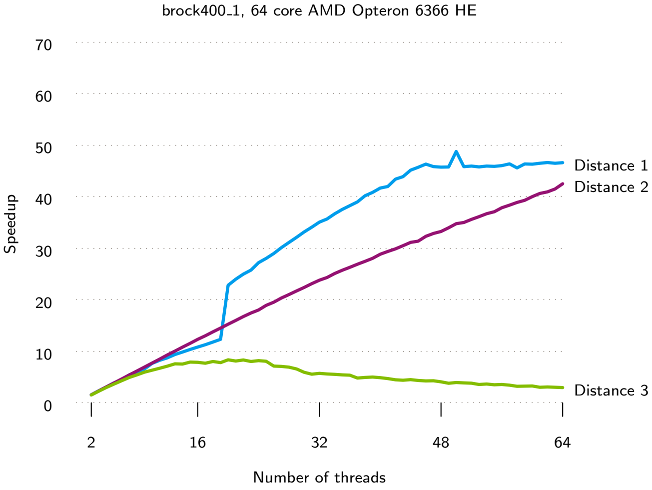

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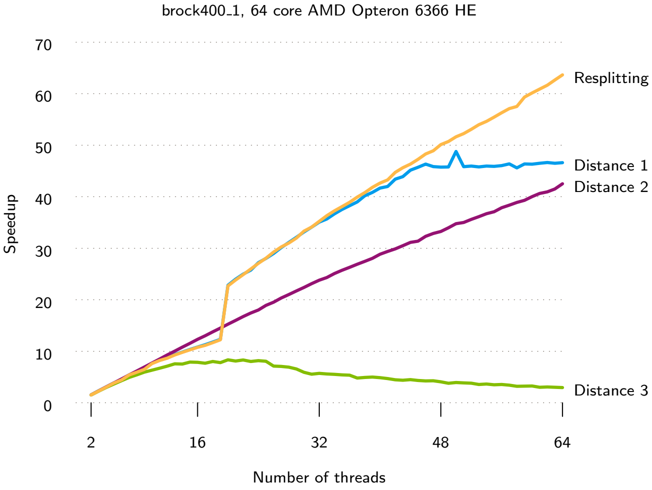

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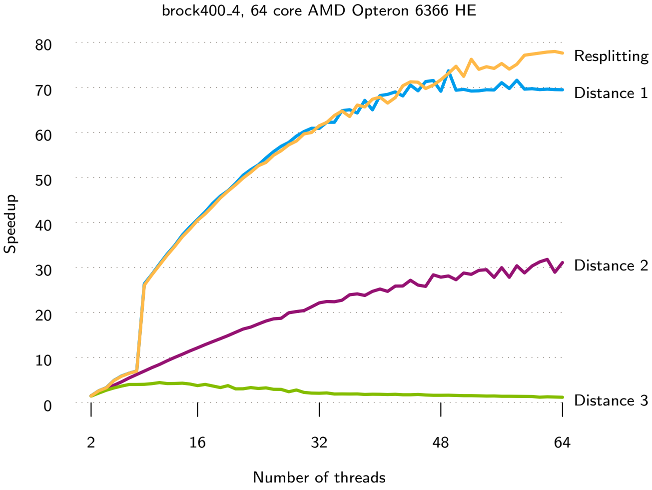

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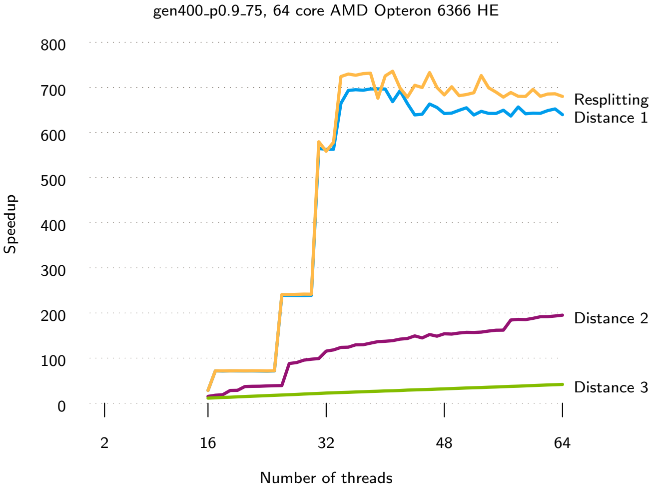


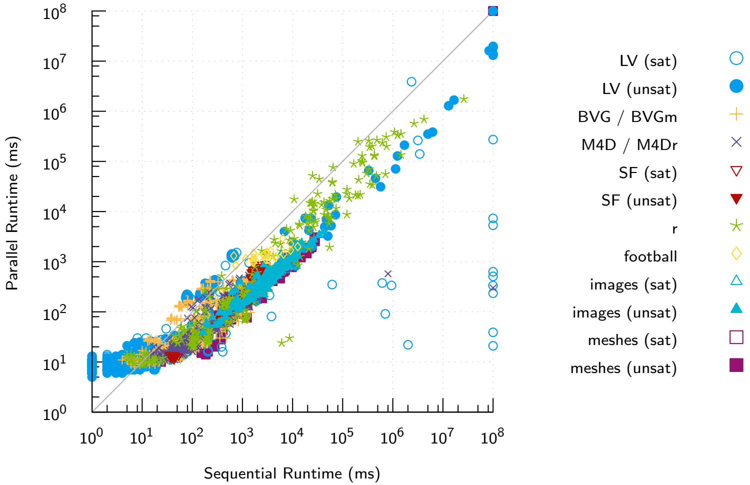
Parallel Search Order Matters

- Value-ordering heuristics tend to be **worst high up** the search tree.
- But depth-first searches commit completely to the first choice made. . .
- Discrepancy searches can avoid this problem by doing more work in total. Parallel search can give **similar benefits for free**.

Safety and Reproducibility

- My “wish list”:
  1. Parallel search should **not be substantially slower** than sequential search.
  2. Adding more processors should **not make things substantially worse**.
  3. Running the same program twice on the same hardware should give **similar runtimes**.
- This is surprisingly tricky.
- On top of all that, we want to **prioritise work stealing** from where we’re most likely to be wrong, or possibly from where we’re most likely not to eliminate a subtree.

Parallel Search is Worth Doing



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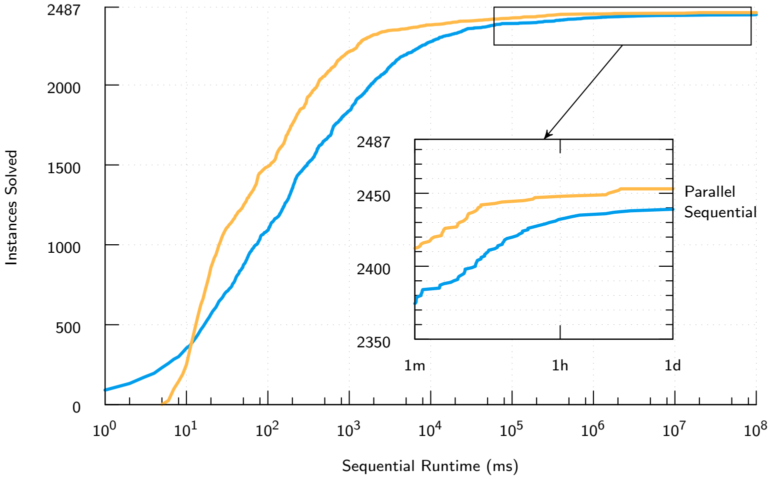

Describing and Implementing Parallel Search

- Implementing safe and reproducible parallel search by hand, even just for multi-core, is painful.
- Current high level approaches don't offer the properties we need.
- Is there a better way?

Symmetries

- Some graphs have known symmetries. Can we exploit this?
  - In some ways, maximum clique is just a completely symmetric version of maximum common subgraph.
- What about if we have to detect the symmetries ourselves dynamically?

Explaining Failures

- Backjumping works because when we fail, we **work out why**, and use that to backtrack further.
- But then we throw that information away...
- CNF encodings for graph problems tend to be annoyingly big, and lose structural information.

Graph Algorithms and Optimisation

- There are a lot of real-world optimisation problems involving **a graph problem** (subgraph isomorphism, subgraph covering, finding sequences of related subgraphs, clique finding, graph colouring, . . .), plus some **other constraints**.
- Can we make these problems easier to specify in a **high-level constraint modelling language** like ~~Essence'~~ MiniZinc?
- There is a continuum of what we could do with these models:
  - Compile to CP, MIP or SAT (but these models tend to be large, and lose structural and heuristic information).
  - A hybrid, multi-solver approach, "graph morphisms modulo theories" style (but we need better theories).
  - Compile to subgraph isomorphism (but even simple arithmetic constraints become disgusting under reduction).

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