Subgraph Isomorphism in Practice

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in conspiracy with Blair Archibald, Fraser Dunlop, Stephan Gocht, Ruth Hoffmann, Jakob Nordström, Patrick Prosser, Christine Solnon and James Trimble

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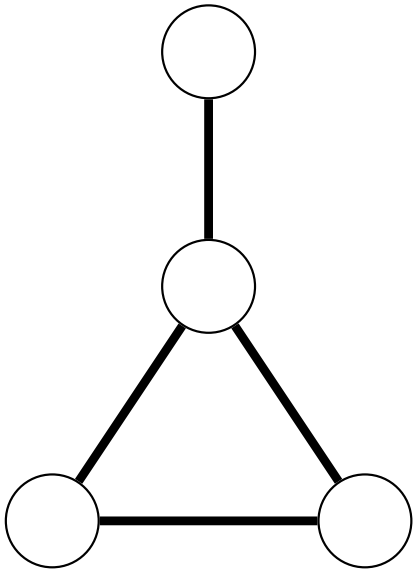
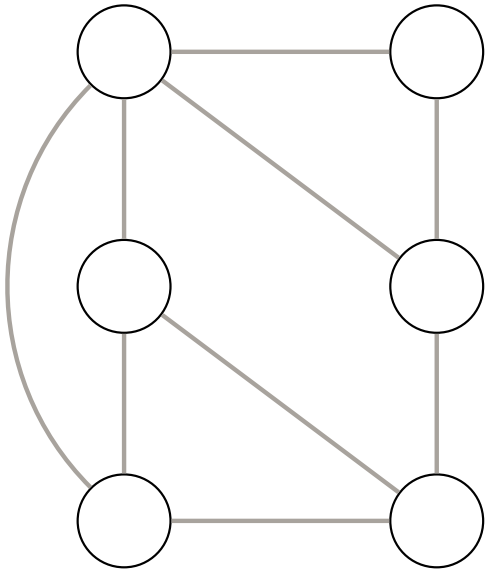
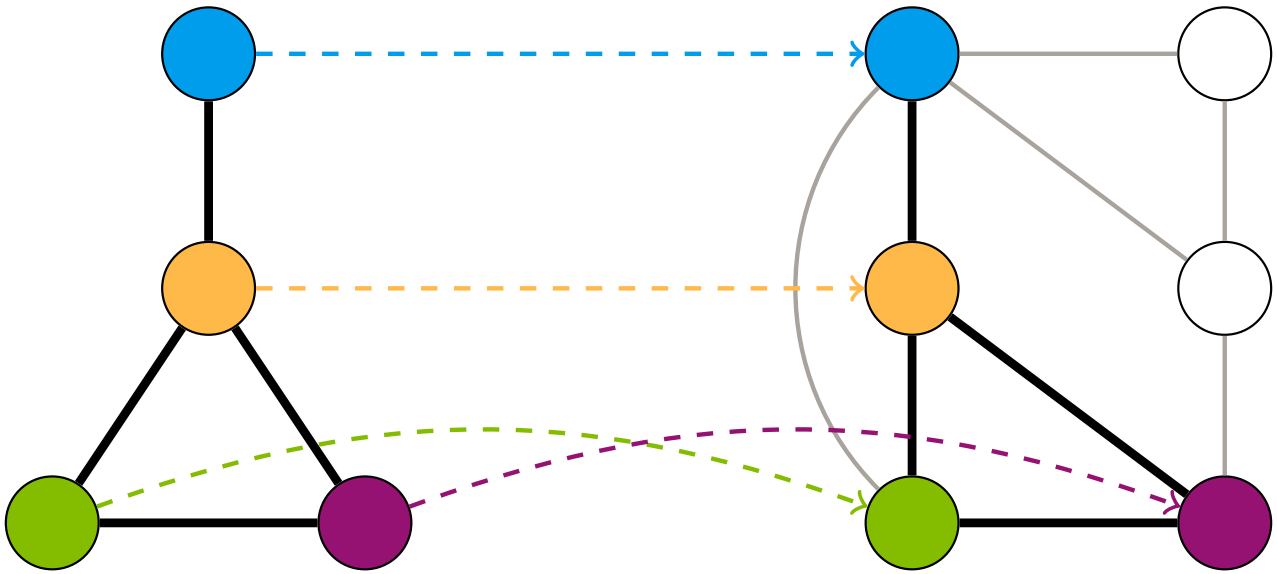
Subgraph Isomorphism

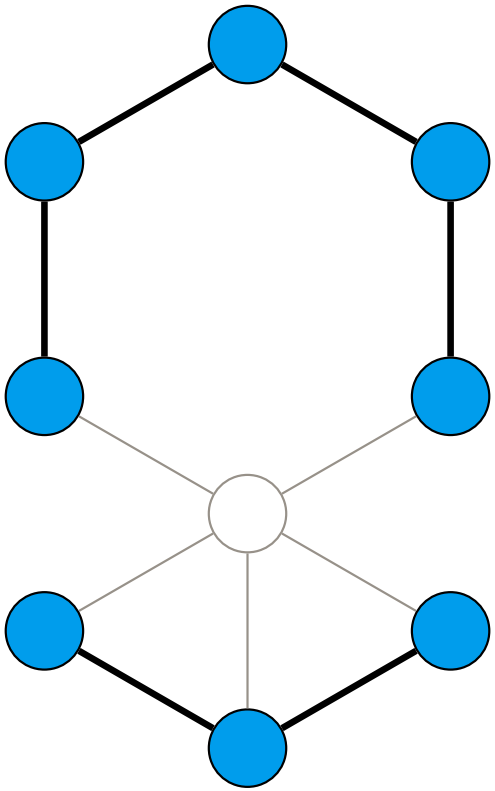


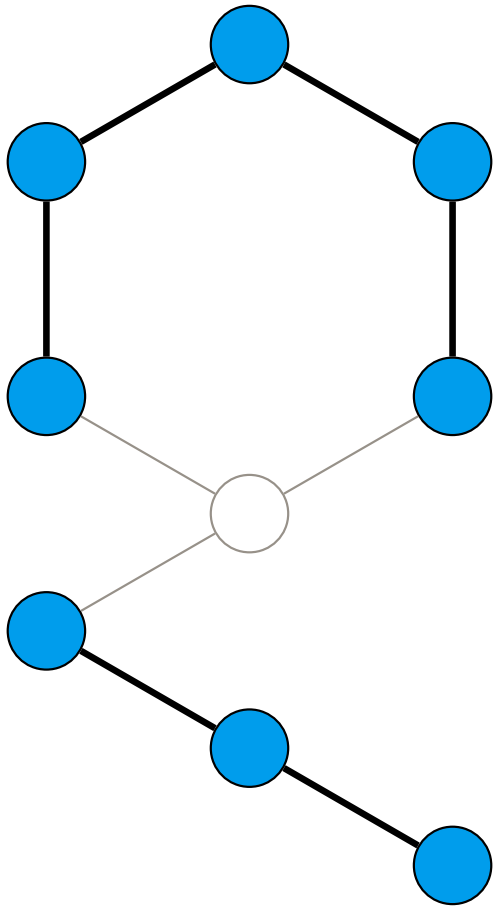


Subgraph Isomorphism

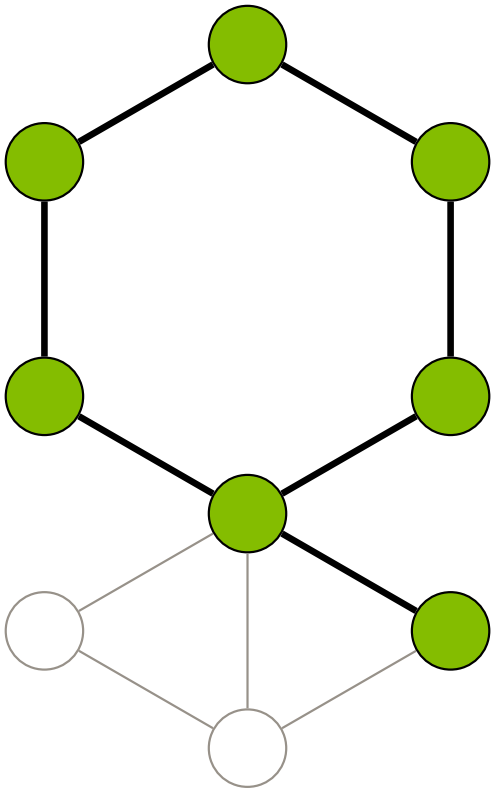


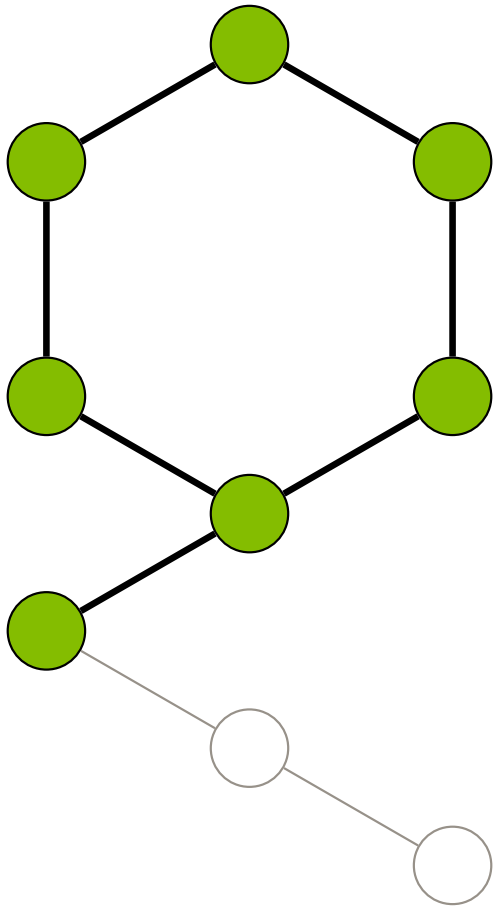
Maximum Common Induced Subgraph



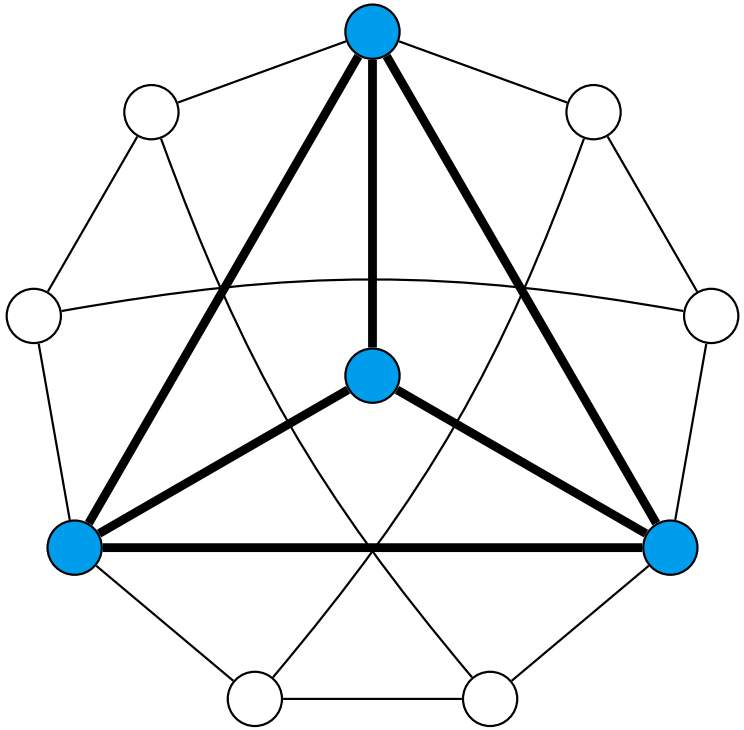


Maximum Common Induced Connected Subgraph





Maximum Clique



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.
- 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…

[1] Terms and conditions apply.

Subgraph Isomorphism, as a Constraint Program

- A variable for each pattern vertex. The domains are all of the target vertices.
- At least two sets of constraints:
  - Adjacent pairs of vertices must be mapped to adjacent pairs of vertices.
  - All different.
- Then we get clever:
  - Extra constraints about degrees, paths, ...
  - Better data structures and propagation queues.
  - Very good variable- and value-ordering heuristics.

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

Benchmark Instances

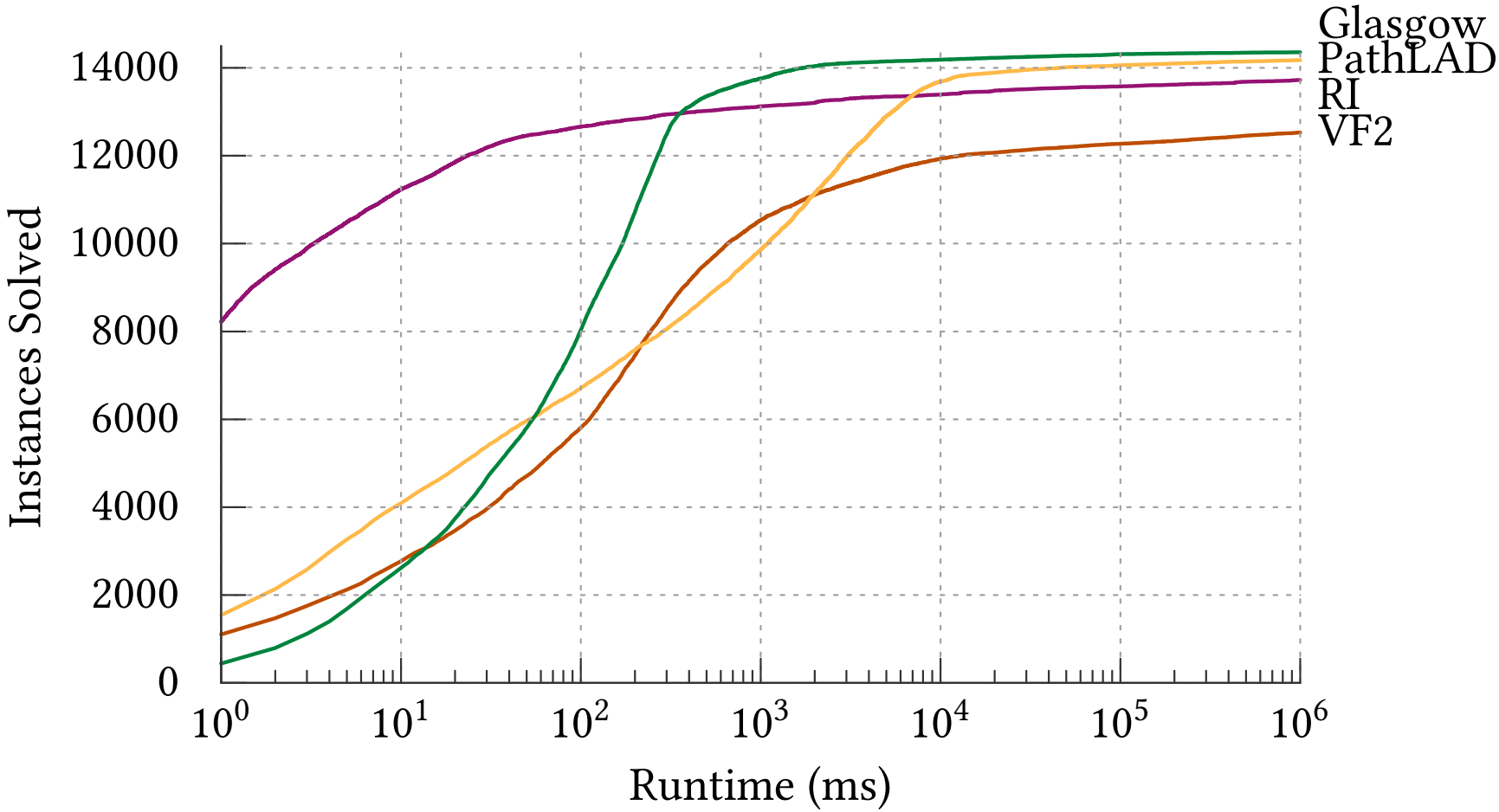
- 14,621 instances from Christine Solnon's collection:
  - Randomly generated with different models.
  - Real-world graphs.
  - Computer vision problems.
  - Biochemistry problems.
  - Phase transition instances.
- At least...
  - $\geq$ 2,110 satisfiable.
  - $\geq$ 12,322 unsatisfiable.
- A lot of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

Hardware

- HPC, optimised for throughput not reproducibility.[2]
- Dual Intel Xeon E5-2695 v4 CPUs, 2×18 cores
- 256GBytes RAM
- GCC 7.2.0
- C++ native threads, SGI MPT MPI

[2]This work used the Cirrus UK National Tier-2 HPC Service at EPCC (http://www.cirrus.ac.uk) funded by the University of Edinburgh and EPSRC (EP/P020267/1)

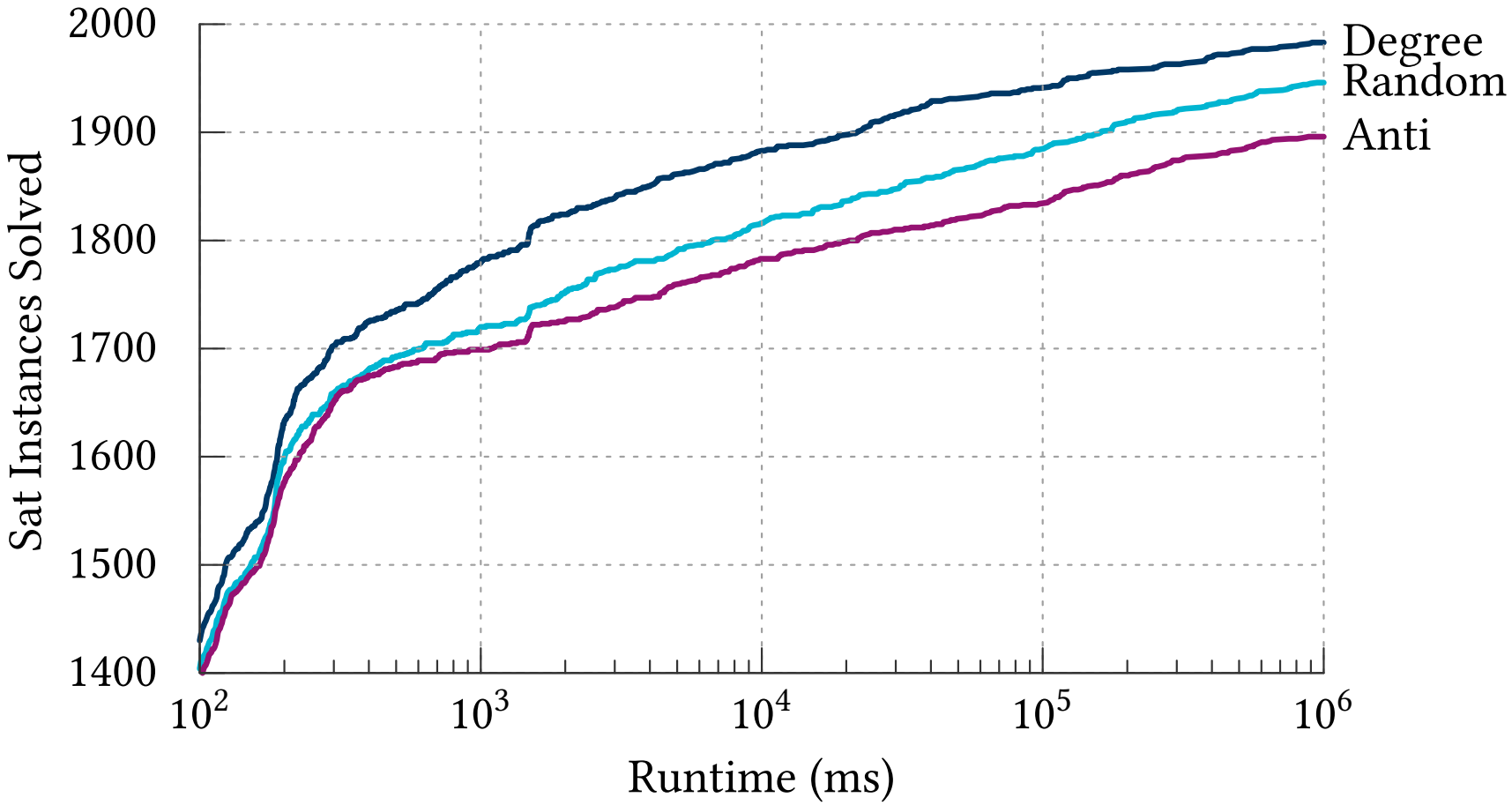
Is It Any Good?



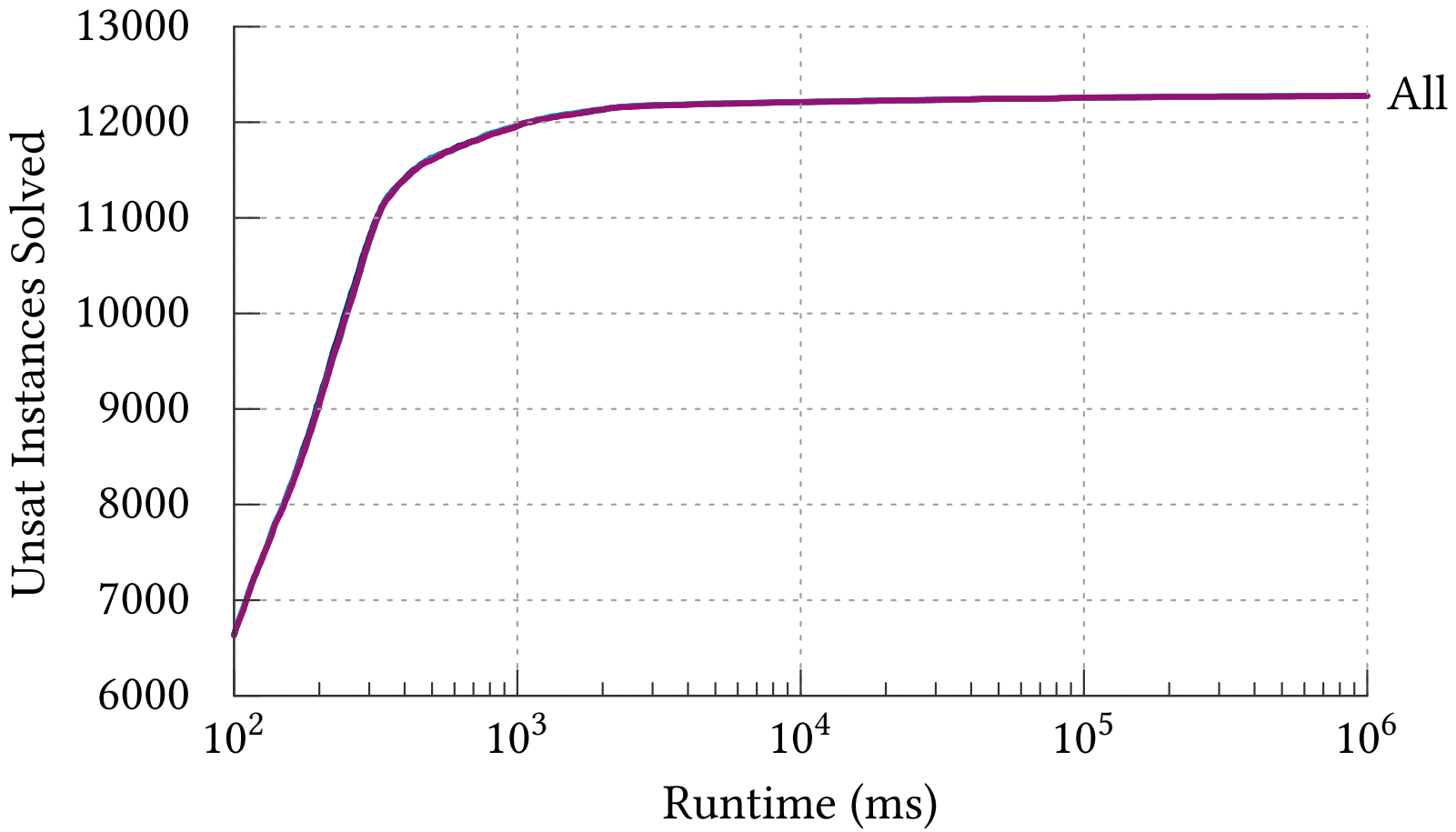
Search Order

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

Sanity Check



Sanity Check



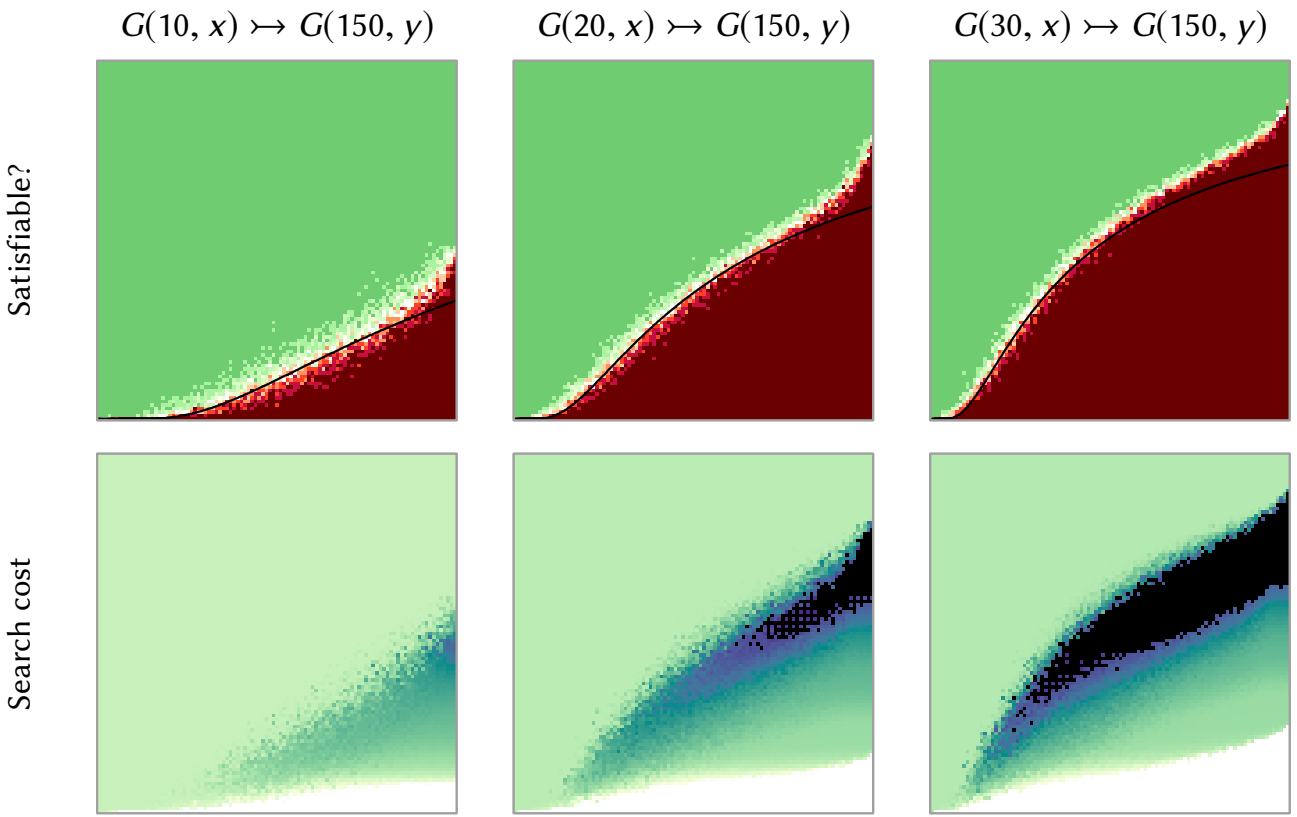
Hand-Wavy Theoretical Justification

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

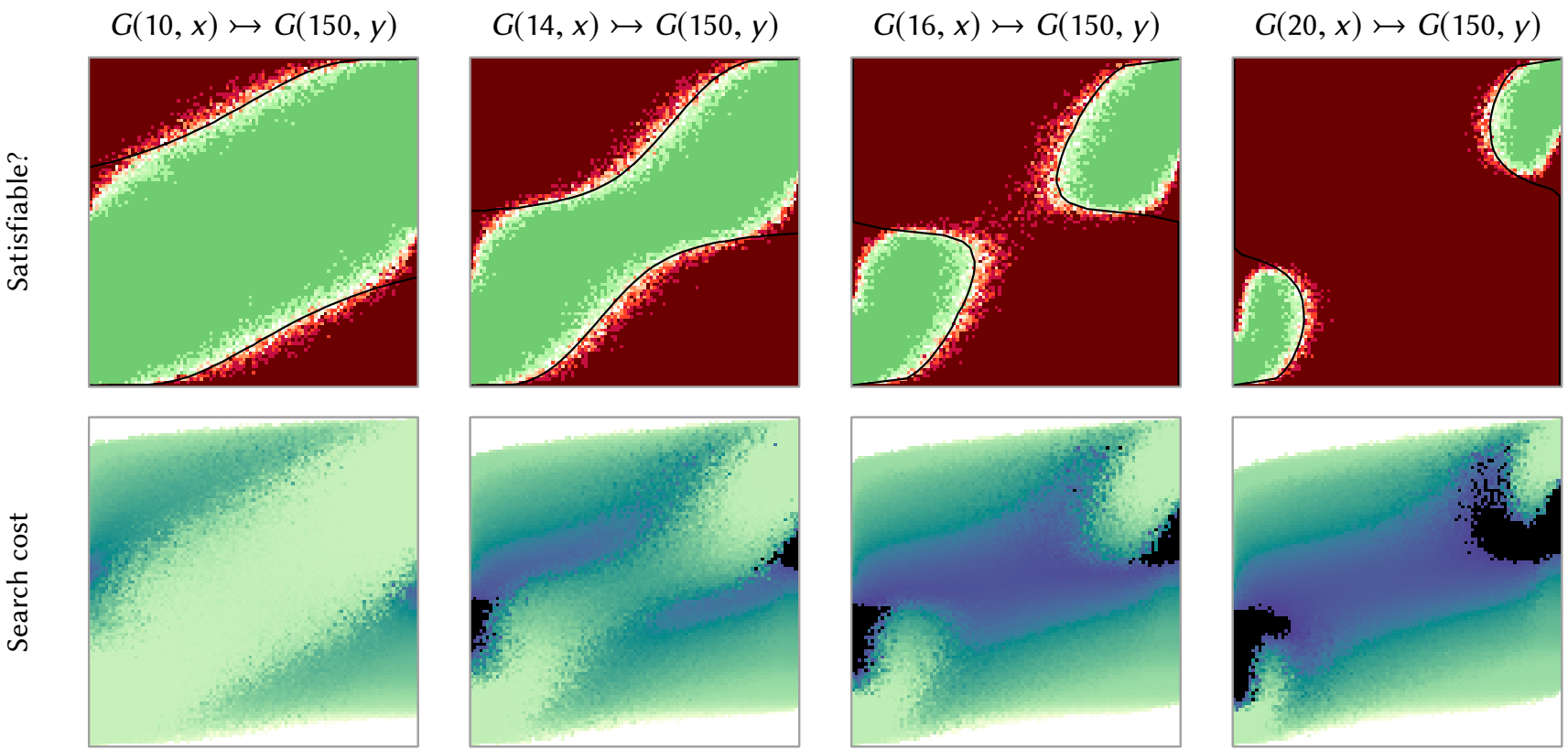
$$\langle Sol \rangle = \underbrace{t \cdot (t-1) \cdot \ldots \cdot (t-p+1)}_{\text{injective mapping}} \cdot \underbrace{u^{q \cdot \binom{p}{2}}}_{\text{adjacency}}$$

- 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.

Subgraph Isomorphism in Random Graphs



Induced Subgraph Isomorphism is More Complicated...



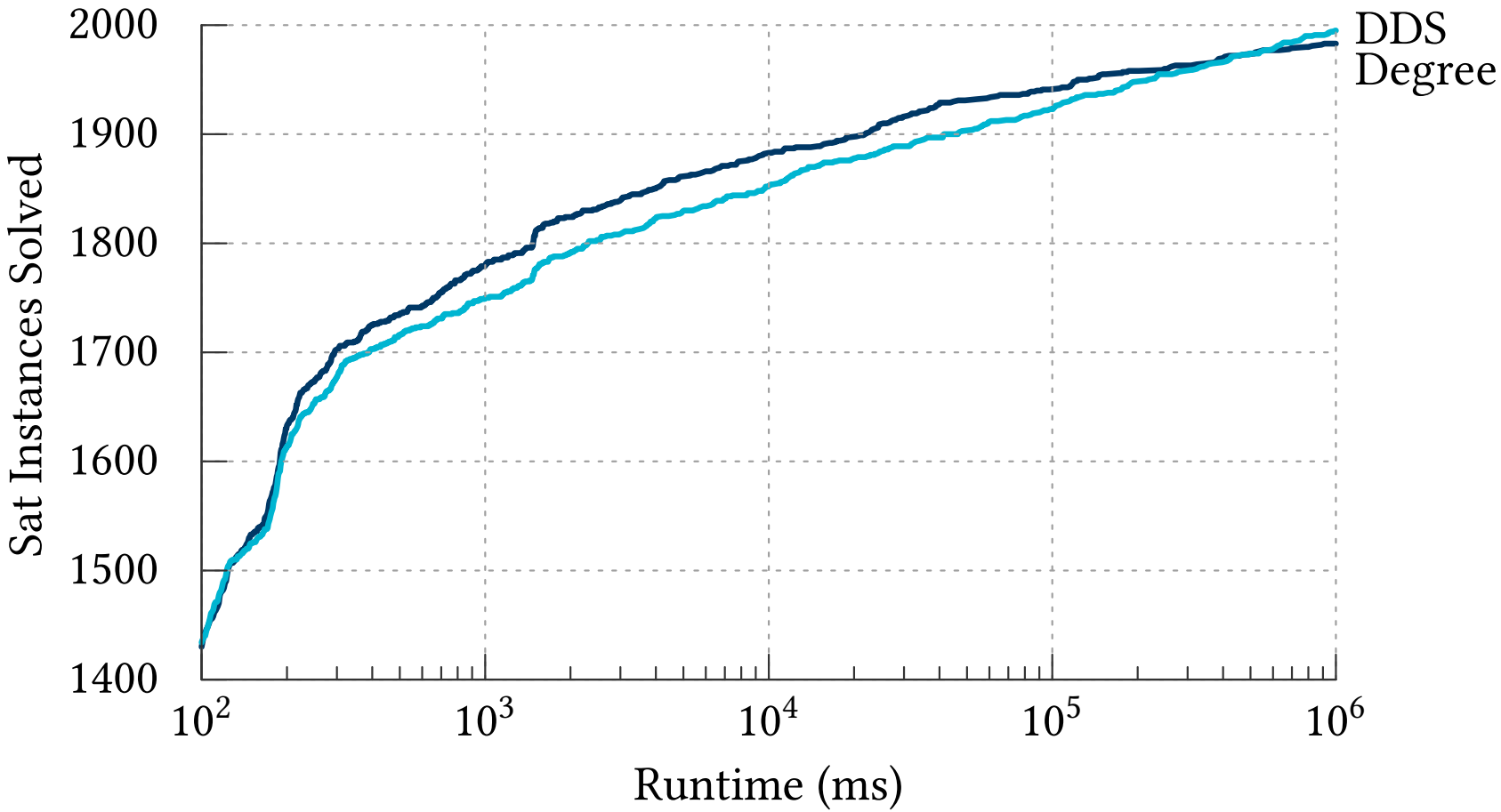
Back to Value-Ordering Heuristics

- 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?



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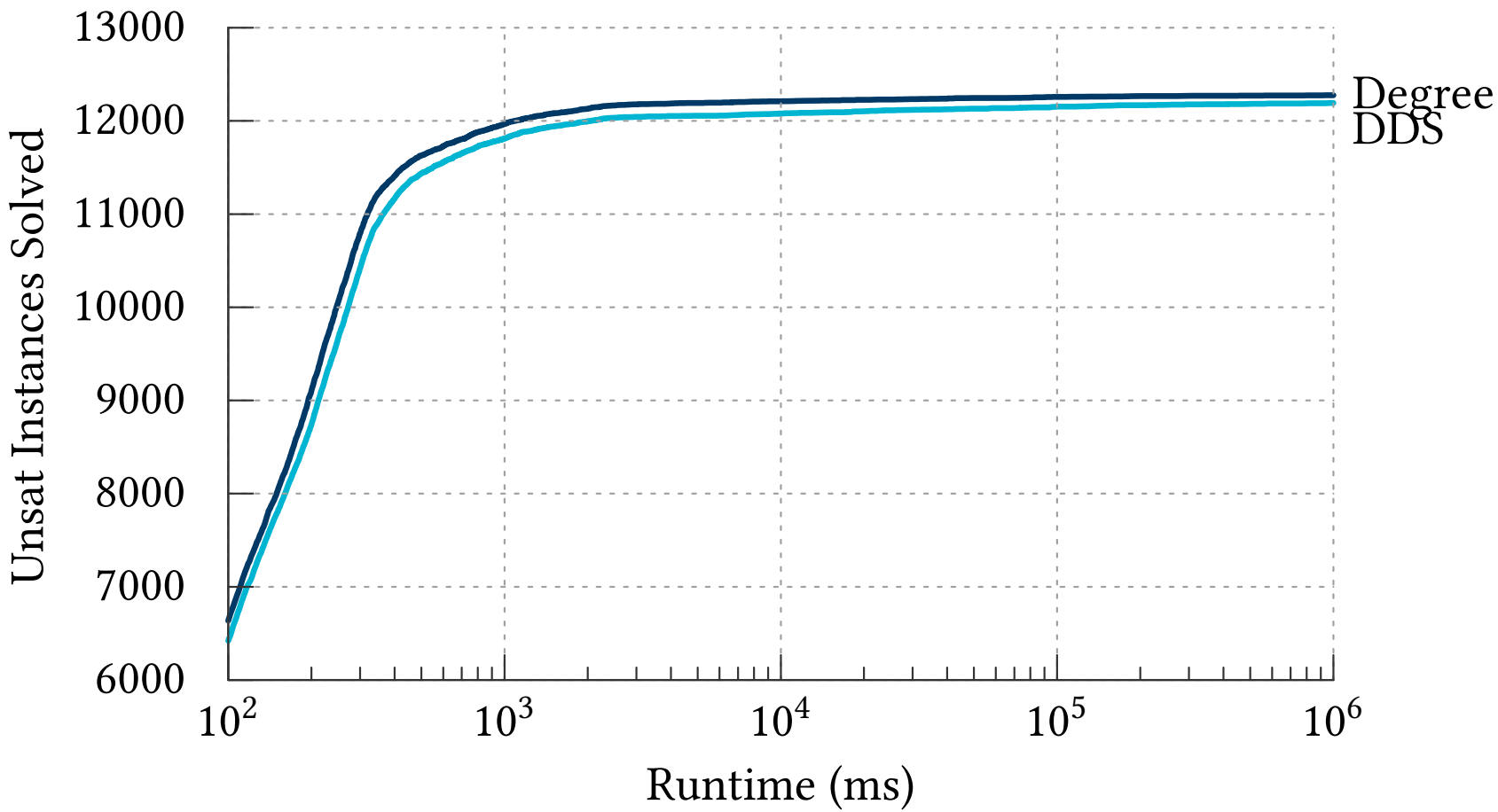

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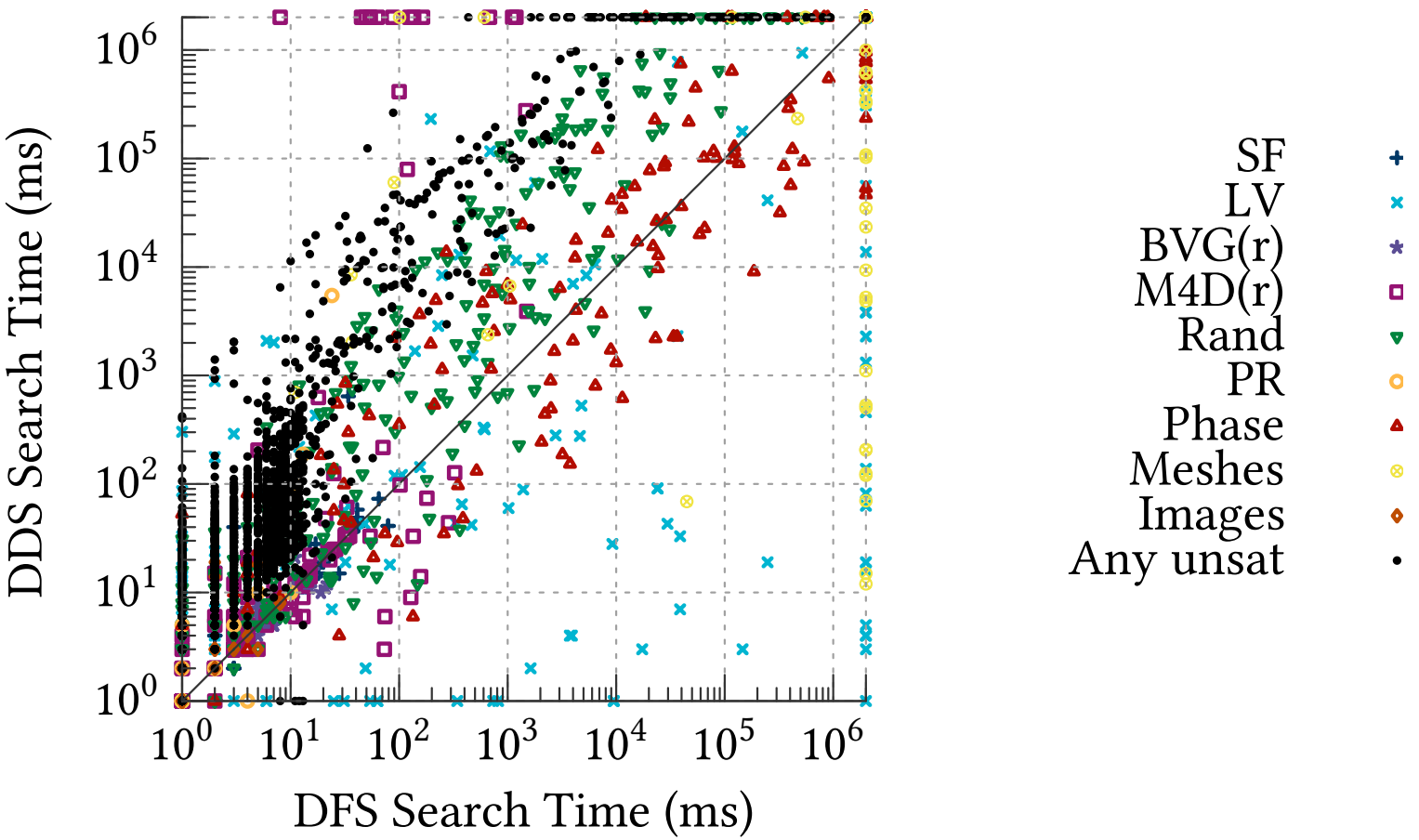
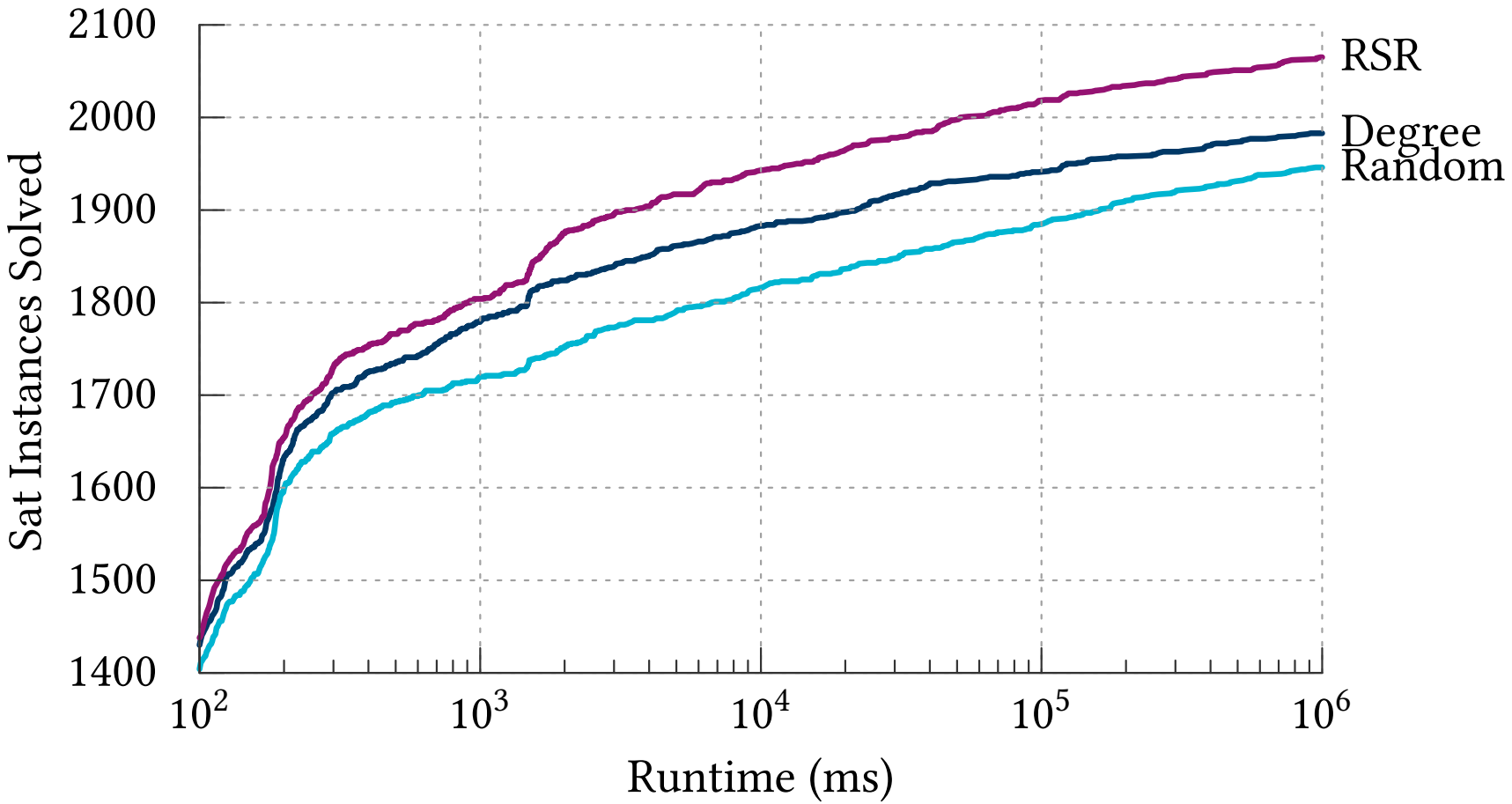


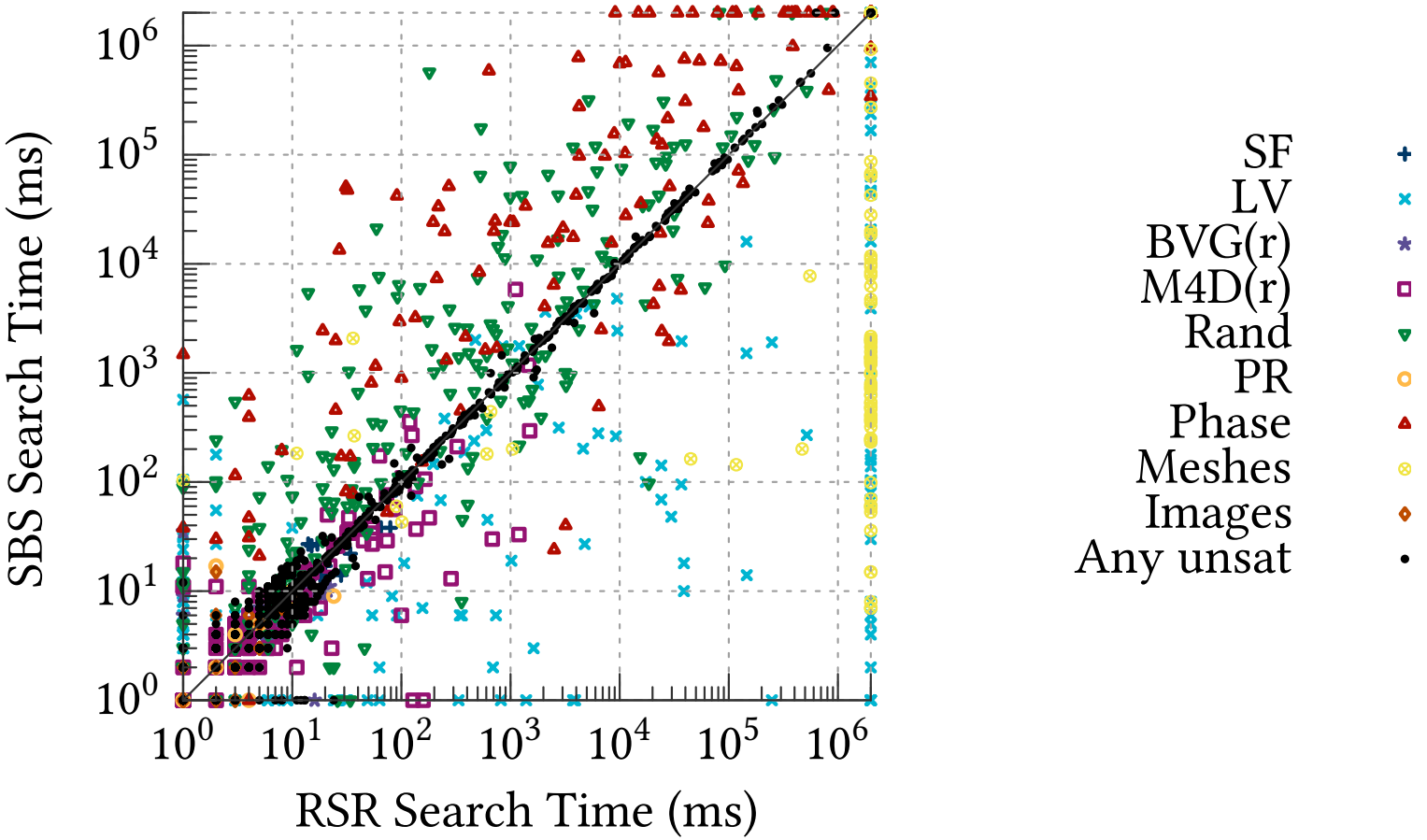
Random Search with Restarts and Nogood Recording

- 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



Random Search with Restarts and Nogood Recording



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.

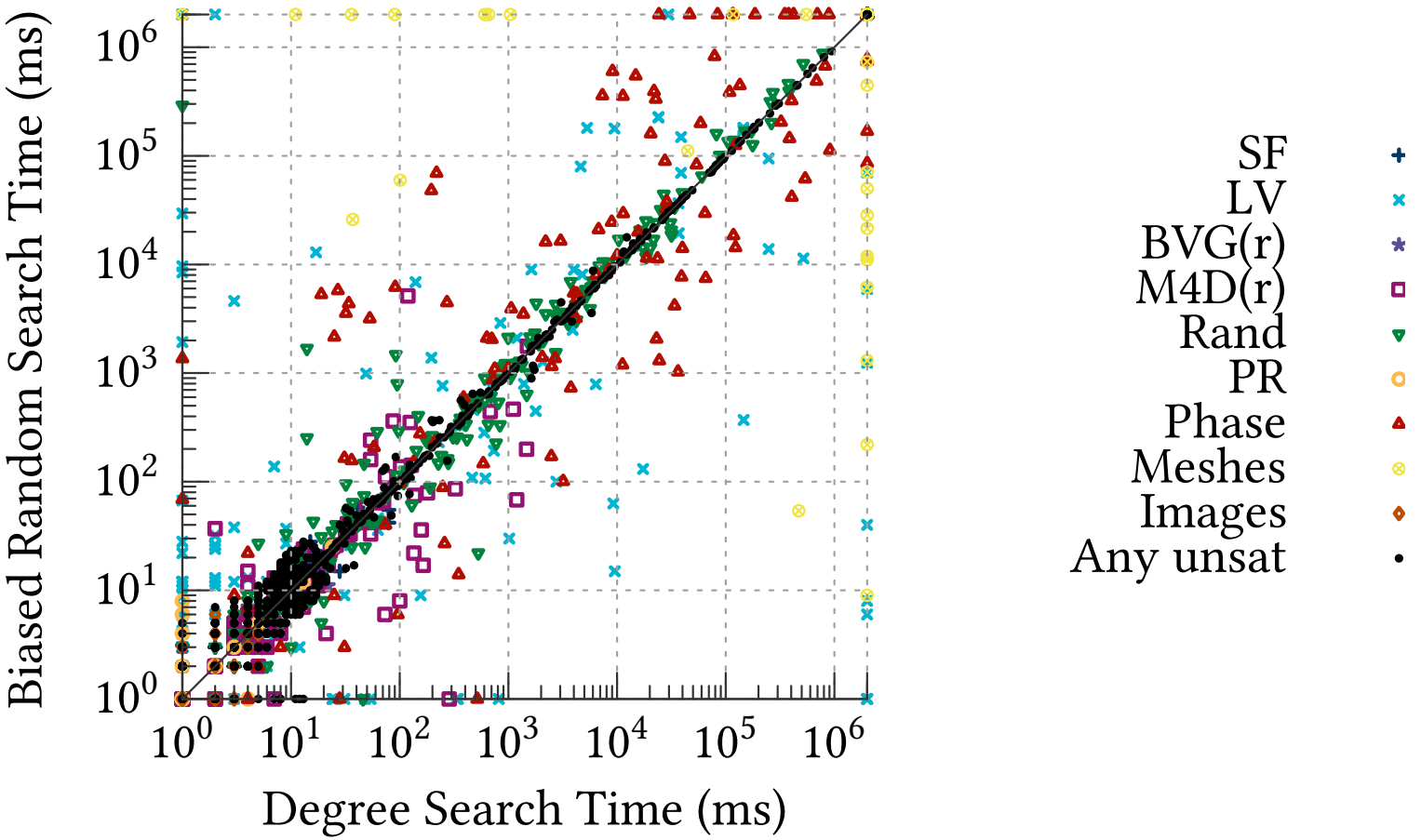
A Slightly Random Value-Ordering Heuristic

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

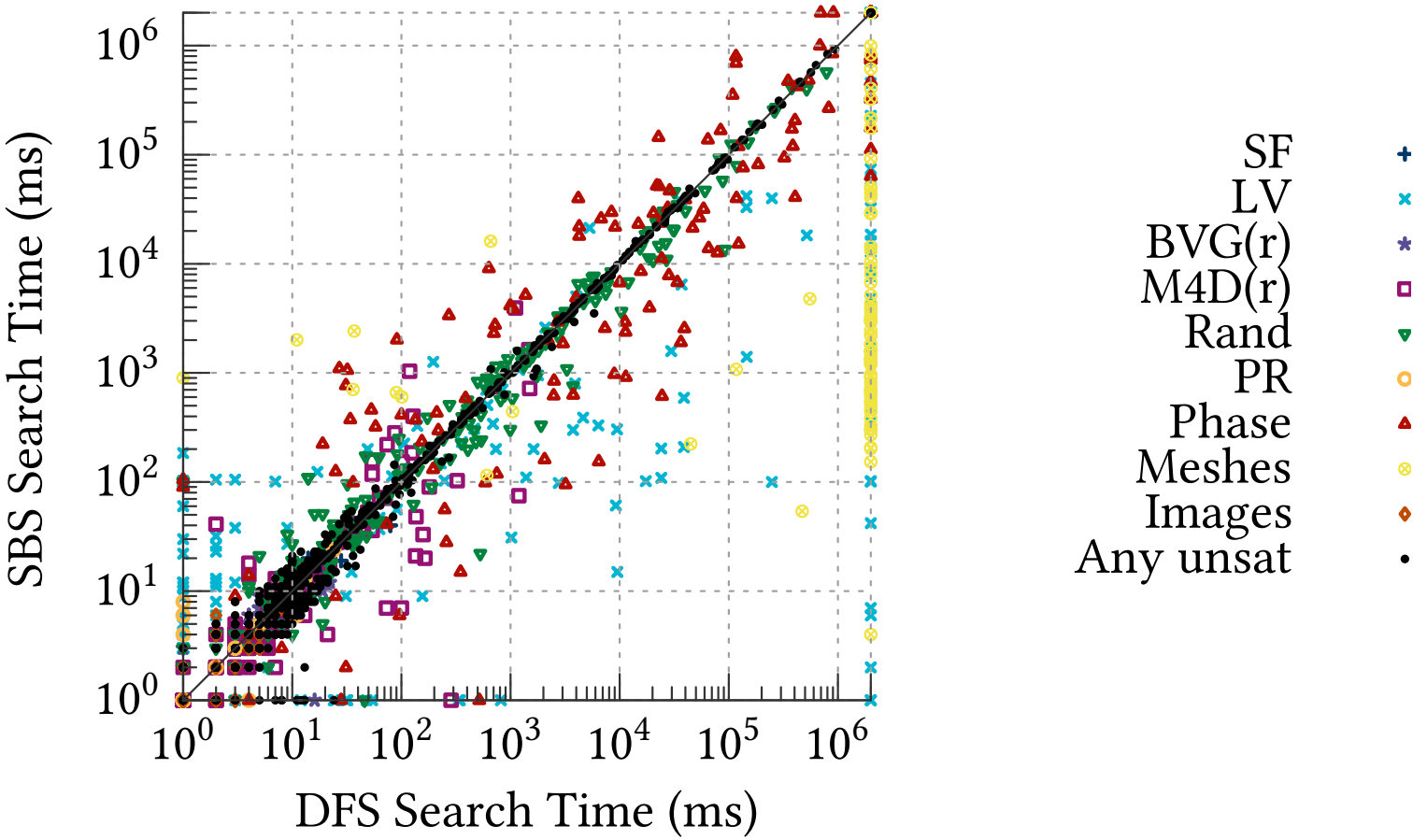
$$p(v') = \frac{2^{\deg(v')}}{\sum_{w \in D_v} 2^{\deg(w)}}$$

- 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.

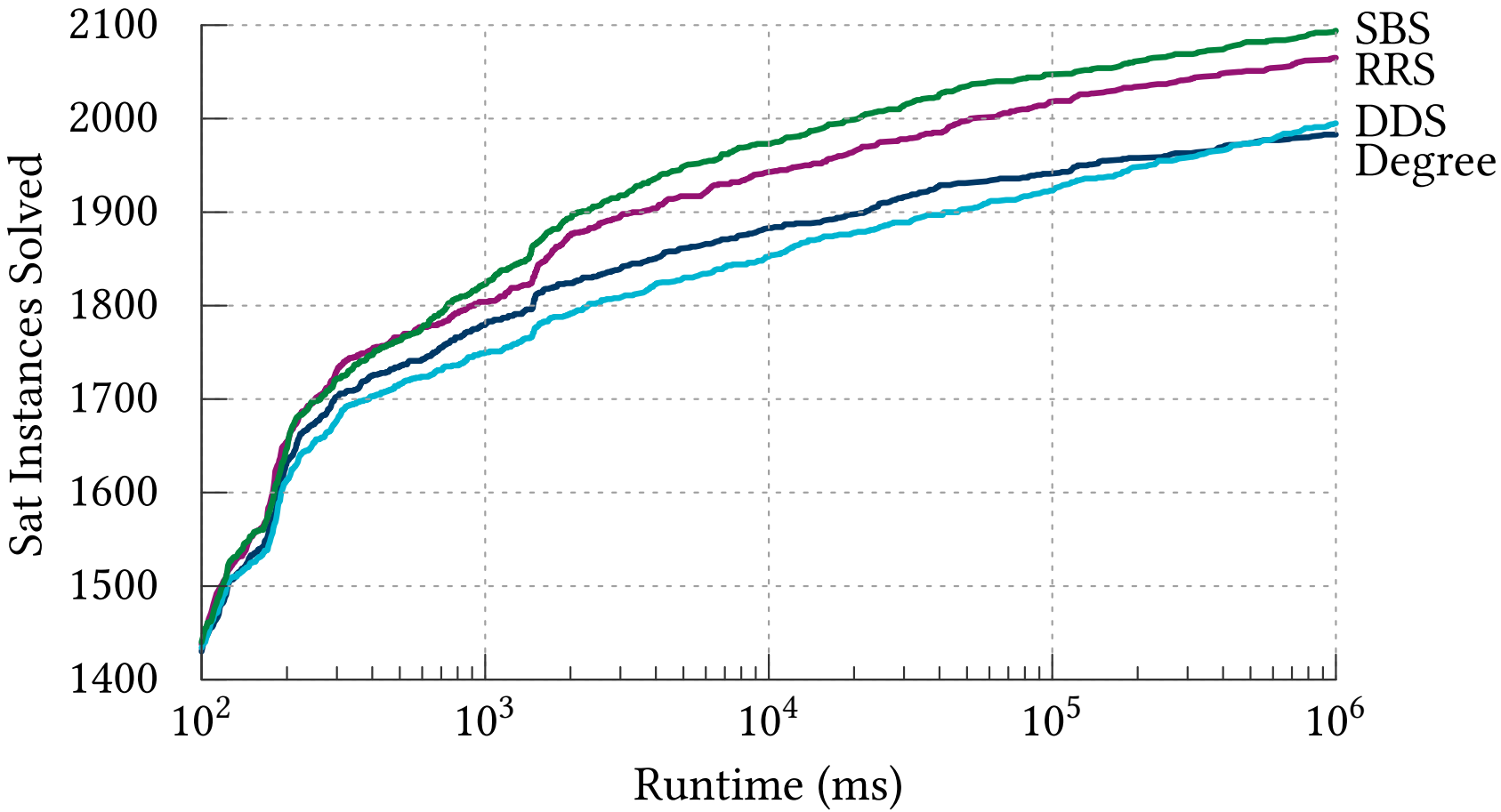
A Slightly Random Value-Ordering Heuristic



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

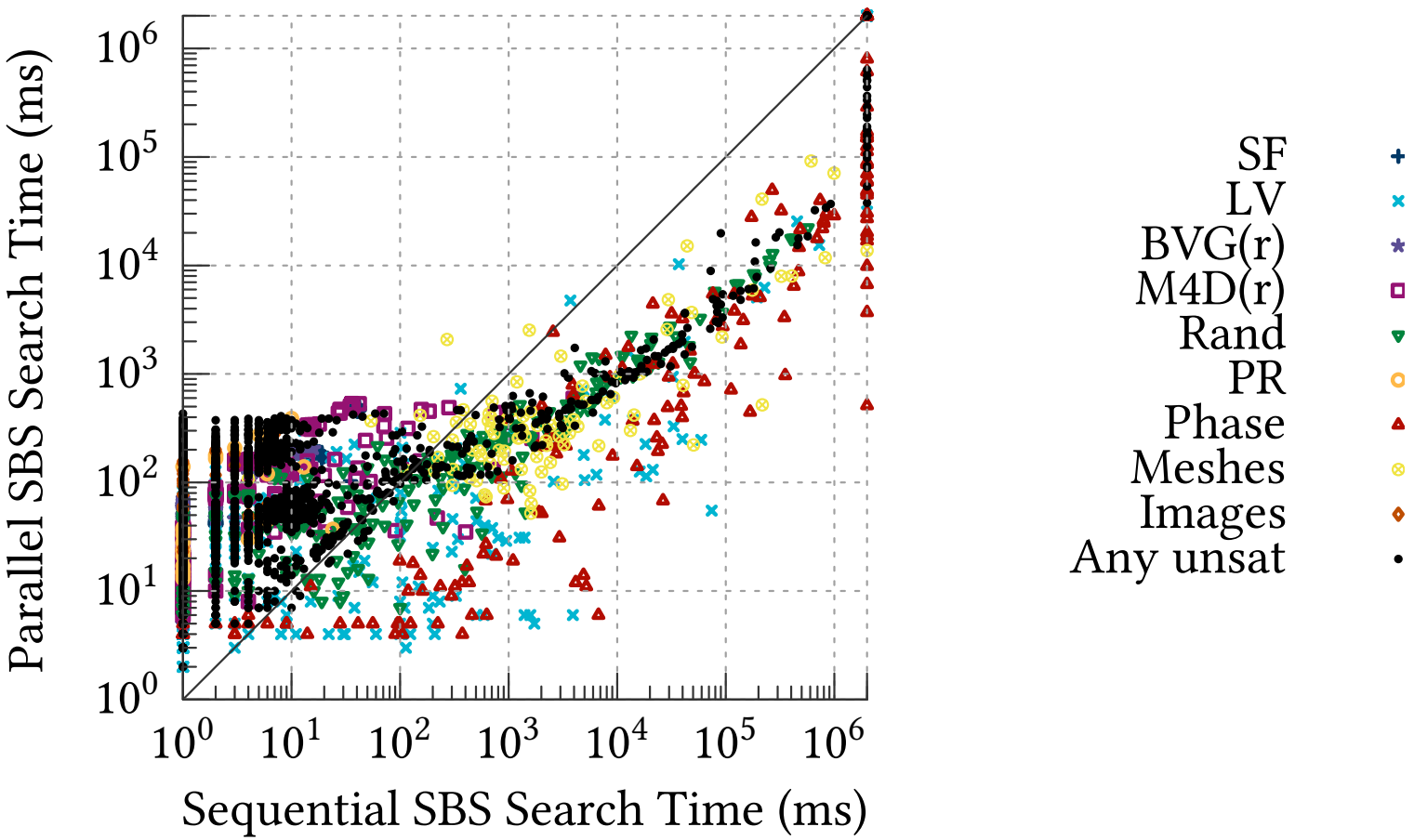
Is It Better?


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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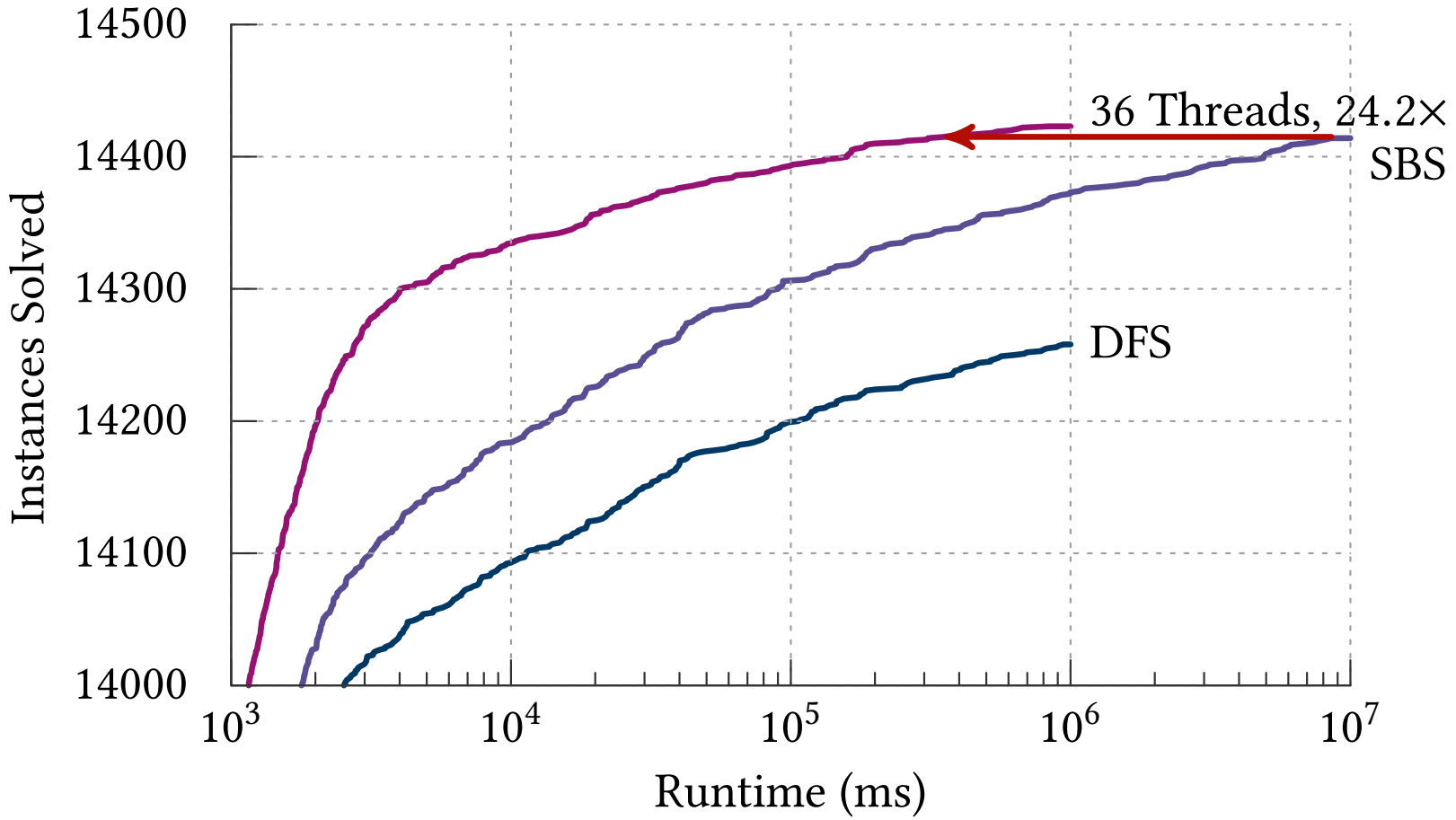

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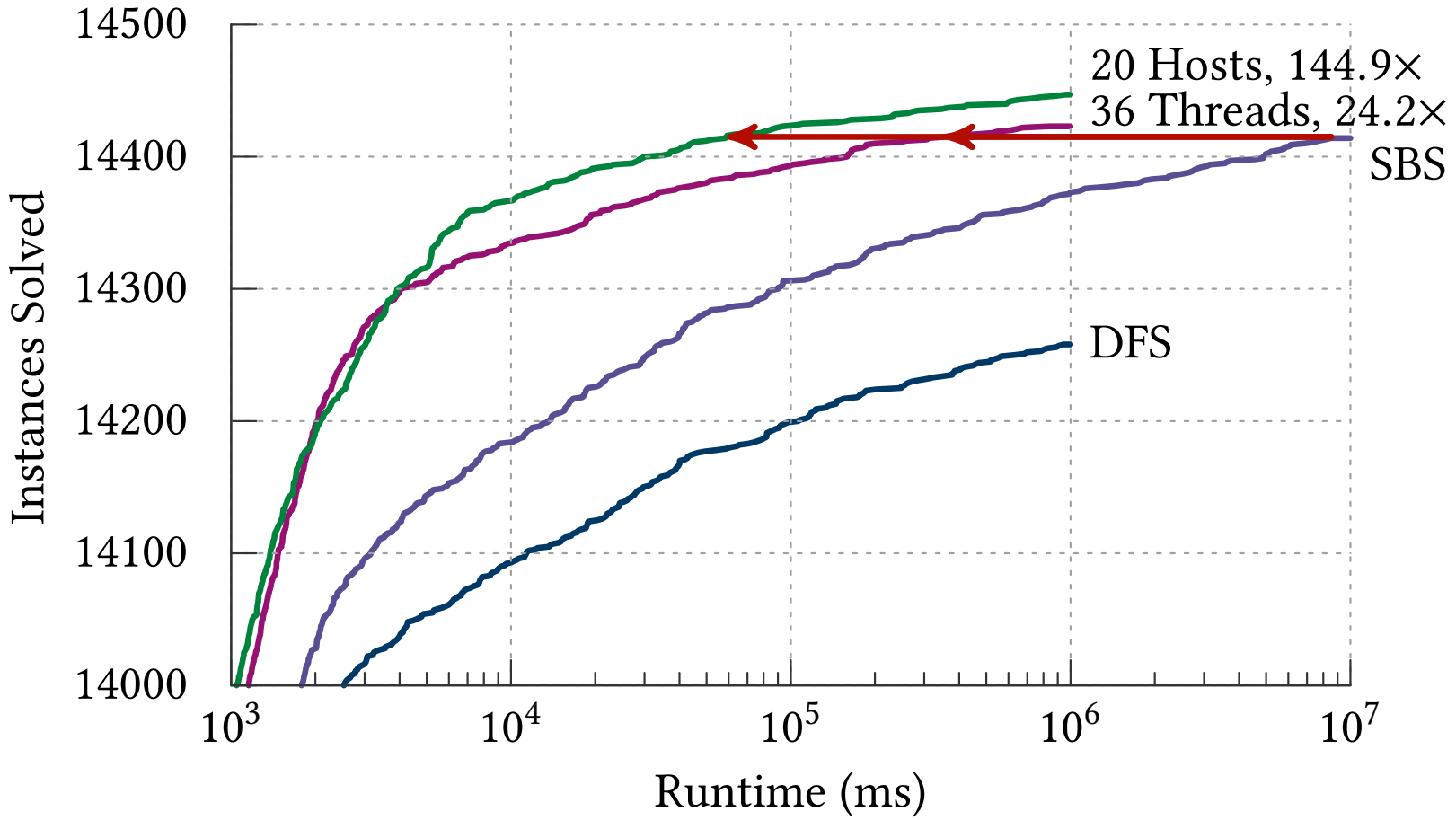

Is There Another Way?

- This approach: assume the inputs are random graphs.
- Another possibility: “From Support Propagation to Belief Propagation in Constraint Programming.”, Gilles Pesant, JAIR 66 (2019).
- At AAAI 2020: “A Learning based Branch and Bound for Maximum Common Subgraph related Problems”, Yanli Liu, Chumin Li, Hua Jiang.

Can You Help?

- Better search
- Conflict analysis
- Symmetries
- Benchmark instances
- Side constraints
- Subgraph counting

Conclusion

- CP can help with designing other algorithms, too.
- Subgraph isomorphism is a nice testbed for learning about CP, because it's just the right amount of complicated.

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