Machine Learning and Logic: Fast and Slow Thinking

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Is Computer Science Fundamentally Changing?

Formal Science vs Data Science

- We are at peak hype about machine learning and big data!
- *Common perception*: A Kuhnian paradigm shift!

– "Throw out the old, bring in the new!"

- *In reality*: new scientific theories *refine* old ones.

– After all, we went to the moon with Newtonian Mechanics!

- *My Thesis*: Data science *refines* formal science!

Logic vs. Machine Learning

Daniel Kahneman, *Thinking, Fast and Slow*, 2011:

- **Machine Learning**: fast thinking, e.g., "Is this a stop sign?"
- **Logic**: slow thinking, e.g., "Do you stop at a stop sign?"
  - Logic is about semantics!

Example–Autonomous Vehicles: how to establish safety? [Shashua, '17]

- *Data Driven*: Drive 1B miles!
- *Data+Model Driven*: Combine data (1M miles) with reasoning.

Grand Challenge: Combine logic with machine learning!

Regulating Automated Decisions Systems

James Larus and Chris Hankin, CACM, Aug. 2018: "The widespread adoption of AD systems will be economically disruptive and will raise new and complex societal challenges. . . . Disdain for regulation is pervasive throughout the tech industry. In the case of automated decision making, this attitude is mistaken."

How to Regulate?

- Fairness, accountability, transparency, *explainability*

Explainability

Explainable AI: AI in which the results of the solution can be understood by humans – explainable AI is a must for *human-centered AI*.

Corollary: Explanation must be high level, rather than low level – *logic*!

Hermanm Weyl, 1995-1955: "We cannot deny that there lives in us a need for theory that is absolutely inexplicable from a merely phenomenalist standpoint. That need has a drive to create, directed to a symbolic layout of the transcendent, which demands satisfaction."

Grand Challenge: Combine logic with machine learning – *neurosymbolic reasoning*.

My approach: Make logic quantitative.

Boole's Symbolic Logic

Boole's insight: Aristotle's syllogisms are about *classes* of objects, which can be treated *algebraically*.

> "If an adjective, as 'good', is employed as a term of description, let us represent by a letter, as y, all things to which the description 'good' is applicable, i.e., 'all good things', or the class of 'good things'. Let it further be agreed that by the combination xy shall be represented that class of things to which the name or description represented by x and y are simultaneously applicable. Thus, if x alone stands for 'white' things and y for 'sheep', let xy stand for 'white sheep'.

Boolean Satisfiability

Boolean Satisfiability (SAT); Given a Boolean expression, using "and" ($\wedge$) "or", ($\vee$) and "not" ($\neg$), *is there a satisfying solution* (an assignment of 0's and 1's to the variables that makes the expression equal 1)?

Example:

$$(\neg x_1 \vee x_2 \vee x_3) \wedge (\neg x_2 \vee \neg x_3 \vee x_4) \wedge (x_3 \vee x_1 \vee x_4)$$

Solution: $x_1 = 0$, $x_2 = 0$, $x_3 = 1$, $x_4 = 1$

Complexity of Boolean Reasoning

History:

- William Stanley Jevons, 1835-1882: "I have given much attention, therefore, to lessening both the manual and mental labour of the process, and I shall describe several devices which may be adopted for saving trouble and risk of mistake."
- Ernst Schröder, 1841-1902: "Getting a handle on the consequences of any premises, or at least the fastest method for obtaining these consequences, seems to me to be one of the noblest, if not the ultimate goal of mathematics and logic."
- Cook, 1971, Levin, 1973: Boolean Satisfiability is NP-complete.

Algorithmic Boolean Reasoning: Early History

- Newell, Shaw, and Simon, 1955: "Logic Theorist"
- Davis and Putnam, 1958: "Computational Methods in The Propositional calculus", unpublished report to the NSA
- Davis and Putnam, JACM 1960: "A Computing procedure for quantification theory"
- Davis, Logemman, and Loveland, CACM 1962: "A machine program for theorem proving"

DPLL Method: Propositional Satisfiability Test

- Convert formula to conjunctive normal form (CNF)
- Backtracking search for satisfying truth assignment
- Unit-clause preference

Modern SAT Solving

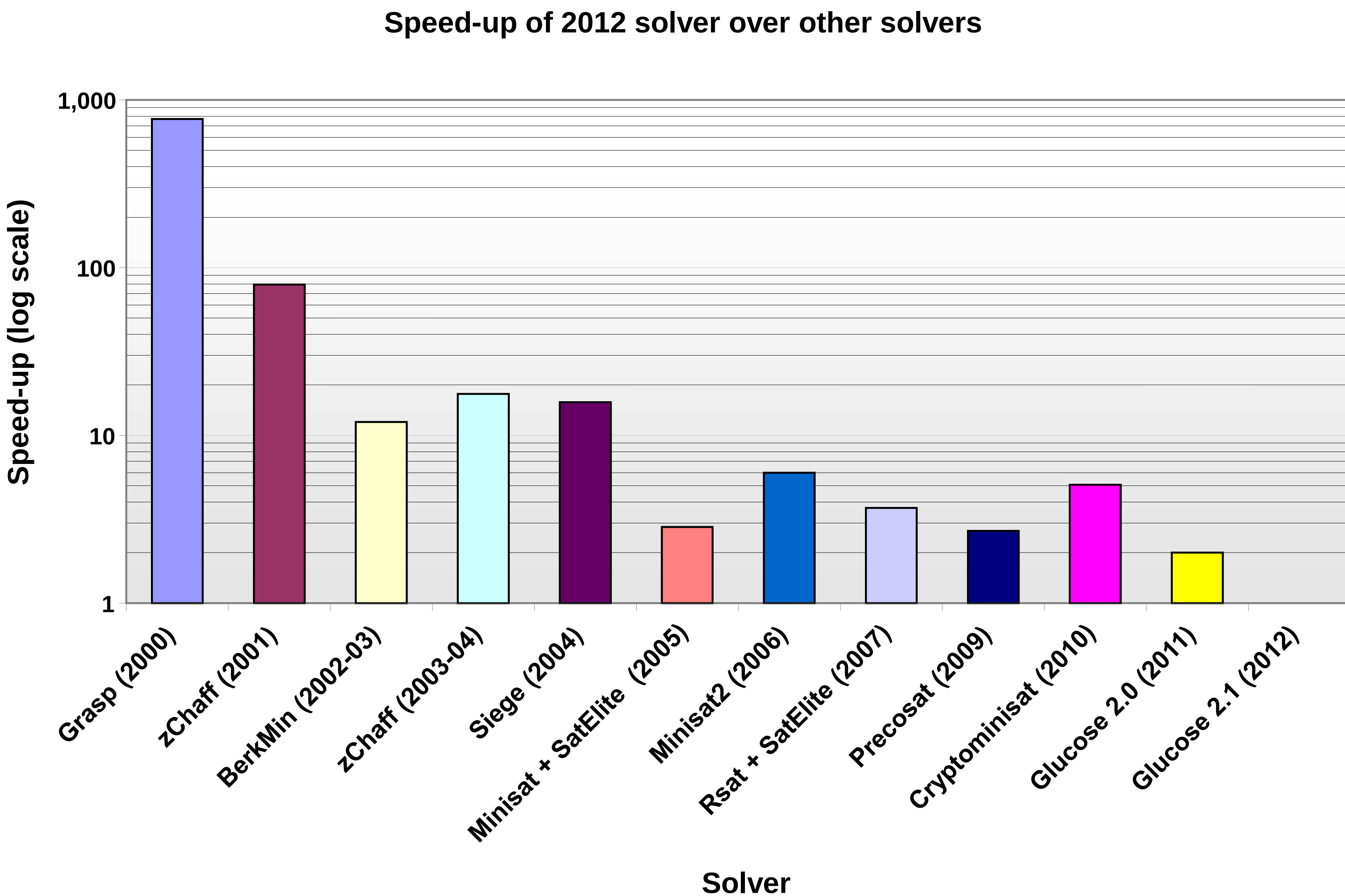
CDCL = conflict-driven clause learning

- Backjumping
- Smart unit-clause preference
- Conflict-driven clause learning
- Smart choice heuristic (brainiac vs speed demon)
- Restarts

Key Tools: GRASP, 1996; Chaff, 2001

Current capacity: *millions* of variables

Some Experience with SAT Solving



Knuth Gets His Satisfaction

SIAM News, July 26, 2016: "Knuth Gives Satisfaction in SIAM von Neumann Lecture"

Donald Knuth gave the 2016 John von Neumann lecture at the SIAM Annual Meeting. The von Neumann lecture is SIAM's most prestigious prize.

Knuth based the lecture, titled "Satisfiability and Combinatorics", on the latest part (Volume 4, Fascicle 6) of his The Art of Computer Programming book series. He showed us the first page of the fascicle, aptly illustrated with the quote "I can't get no satisfaction," from the Rolling Stones. In the preface of the fascicle Knuth says "The story of satisfiability is the tale of a triumph of software engineering, blended with rich doses of beautiful mathematics".

Applications of SAT Solving in SW Engineering

Leonardo De Moura+Nikolaj Björner, 2012: Applications of Z3 at Microsoft

- Symbolic execution
- Model checking
- Static analysis
- Model-based design
- ...

Verification of HW/SW systems

HW/SW Industry: \$1.5T per year!

Major Industrial Problem: *Functional Verification* – ensuring that computing systems satisfy their intended functionality

- Verification consumes the majority of the development effort!

Two Major Approaches:

- *Formal Verification*: Constructing mathematical models of systems under verification and analyzing them mathematically: $\leq$ 10% of verification effort

- *Dynamic Verification*: simulating systems under different testing scenarios and checking the results: $\geq$ 90% of verification effort

Dynamic Verification

- Dominant approach!
- Design is simulated with input test vectors.
- Test vectors represent different verification scenarios.
- Results compared to intended results.
- **Challenge**: Exceedingly large test space!

Motivating Example: HW FP Divider

$z = x/y$: x, y, z are 128-bit floating-point numbers

Question How do we verify that circuit works correctly?

- Try for all values of x and y?
- 2^{256} possibilities
- Sun will go nova before done! *Not scalable!*

Test Generation

Classical Approach: *manual* test generation - capture intuition about problematic input areas

- Verifier can write about 20 test cases per day: *not scalable!*

Modern Approach: *random-constrained* test generation

- Verifier writes *constraints* describing problematic inputs areas (based on designer intuition, past bug reports, etc.)

- Uses *constraint solver* to solve constraints, and uses solutions as test inputs – rely on industrial-strength constraint solvers!

- Proposed by Lichtenstein+Malka+Aharon, 1994: de-facto industry standard today!

Random Solutions

Major Question: How do we generate solutions *randomly* and *uniformly?*

- *Randomly*: We should not reply on solver internals to chose input vectors; we do not know where the errors are!
- *Uniformly*: We should not prefer one area of the solution space to another; we do not know where the errors are!

Uniform Generation of SAT Solutions: Given a SAT formula, generate solutions uniformly at random, while scaling to industrial-size problems.

Constrained Sampling: Applications

Many Applications:

- Constrained-random Test Generation: discussed above
- Personalized Learning: automated problem generation
- Search-Based Optimization: generate random points of the candidate space
- *Probabilistic Inference*: Sample after conditioning
- . . .

Constrained Sampling – Prior Approaches, I

Theory:

- Jerrum+Valiant+Vazirani: *Random generation of combinatorial structures from a uniform distribution*, TCS 1986 – uniform generation by a randomized polytime algrithm with an Σ_2^p oracle.

- Bellare+Goldreich+Petrank: *Uniform generation of NP-witnesses using an NP-oracle*, 2000 – uniform generation by a randomized polytime algorithm with an NP oracle.

We *implemented* the BPG Algorithm: did not scale above 16 variables!

Constrained Sampling – Prior Work, II

Practice:

- *BDD-based*: Yuan, Aziz, Pixley, Albin: *Simplifying Boolean constraint solving for random simulation-vector generation*, 2004 – poor scalability
- *Heuristics approaches*: MCMC-based, randomized solvers, etc. – good scalability, poor uniformity

Almost Uniform Generation of Solutions

New Algorithm – UniGen: Chakraborty, Fremont, Meel, Seshia, V, 2013-15:

- almost uniform generation by a randomized polytime algorithms with a SAT oracle.
- Based on *universal hashing*.
- Uses an *SMT solver*.
- Scales to millions of variables.
- Enables parallel generation of solutions after preprocessing.

Uniformity vs Almost-Uniformity

- Input formula: φ;   Solution space: $Sol(\varphi)$
- Solution-space size: $\kappa = |Sol(\varphi)|$
- Uniform generation: for every assignment y: Prob$[Output = y]$=$1/\kappa$
- Almost-Uniform Generation: for every assignment y: $\frac{(1/\kappa)}{(1+\varepsilon)} \leq Prob[Output = y] \leq (1/\kappa) \times (1+\varepsilon)$

The Basic Idea

1. Partition $Sol(\varphi)$ into "roughly" equal small cells of appropriate size.

2. Choose a random cell.

3. Choose at random a solution in that cell.

You got random solution almost uniformly!

Question: How can we partition $Sol(\varphi)$ into "roughly" equal small cells without knowing the distribution of solutions?

Answer: *Universal Hashing* [Carter-Wegman 1979, Sipser 1983]

Universal Hashing

Hash function: maps $\{0,1\}^n$ to $\{0,1\}^m$

- Random inputs: All cells are roughly equal (in expectation)

Universal family of hash functions: Choose hash function *randomly* from family

- For *arbitrary* distribution on inputs: All cells are roughly equal (in expectation)

Strong Universality

Universal Family: Each input is hashed *uniformly*, but different inputs might not be hashed *independently*.

$H(n, m, r)$: Family of r-*universal* hash functions mapping $\{0,1\}^n$ to $\{0,1\}^m$ such that every r elements are mapped *independently*.

- *Higher* r: Stronger guarantee on *range of sizes* of cells
- r-*wise universality*: Polynomials of degree $r - 1$

Strong Universality

Key: Higher universality $\Rightarrow$ higher complexity!

- **BGP**: n-universality $\Rightarrow$ all cells are small $\Rightarrow$ uniform generation
- **UniGen**: 3-universality $\Rightarrow$ a random cell is small w.h.p $\Rightarrow$ almost-uniform generation

From tens of variables to millions of variables!

XOR-Based 3-Universal Hashing

- Partition $\{0,1\}^n$ into 2^m cells.
- *Variables*: $X_1, X_2, \ldots X_n$
- Pick every variable with probability $1/2$, XOR them, and equate to 0/1 with probability $1/2$.
  - E.g.: $X_1 + X_7 + \ldots + X_{117} = 0$ (splits solution space in half)
- m XOR equations $\Rightarrow 2^m$ cells
- *Cell constraint*: a conjunction of CNF and XOR clauses

SMT: Satisfiability Modulo Theory

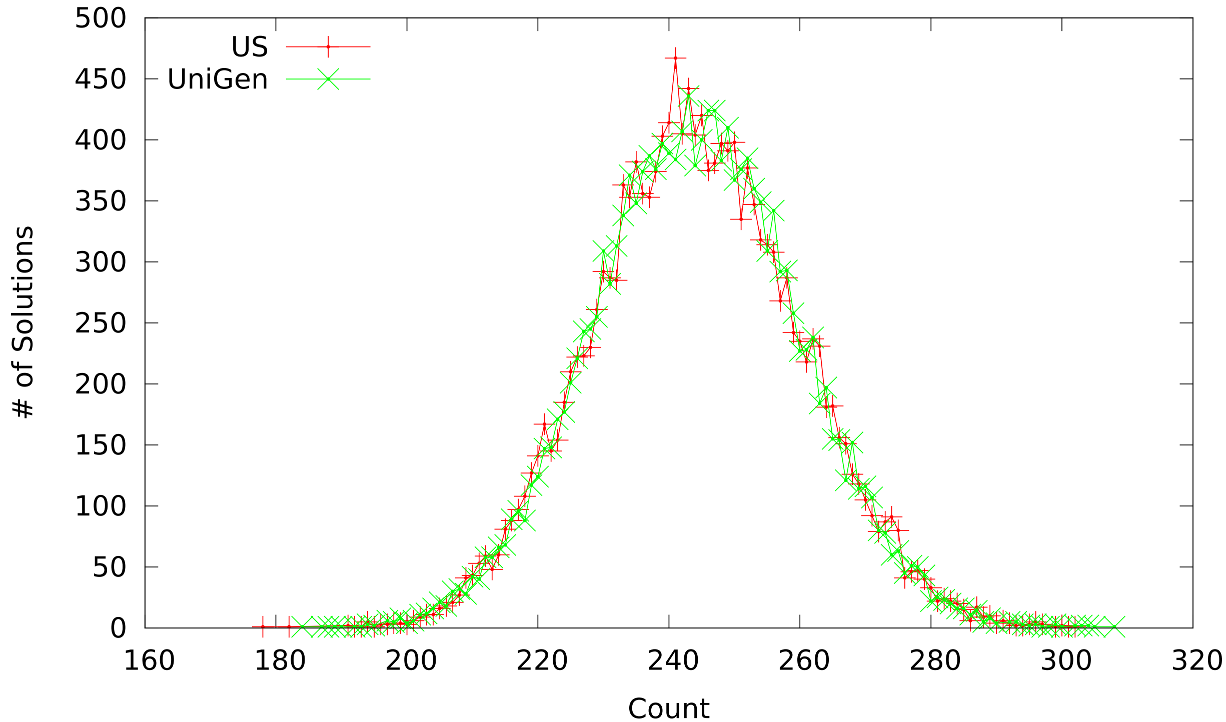
SMT Solving: Solve Boolean combinations of constraints in an underlying theory, e.g., linear constraints, combining SAT techniques and domain-specific techniques.

- Tremendous progress since 2000!

CryptoMiniSAT: M. Soos, 2009

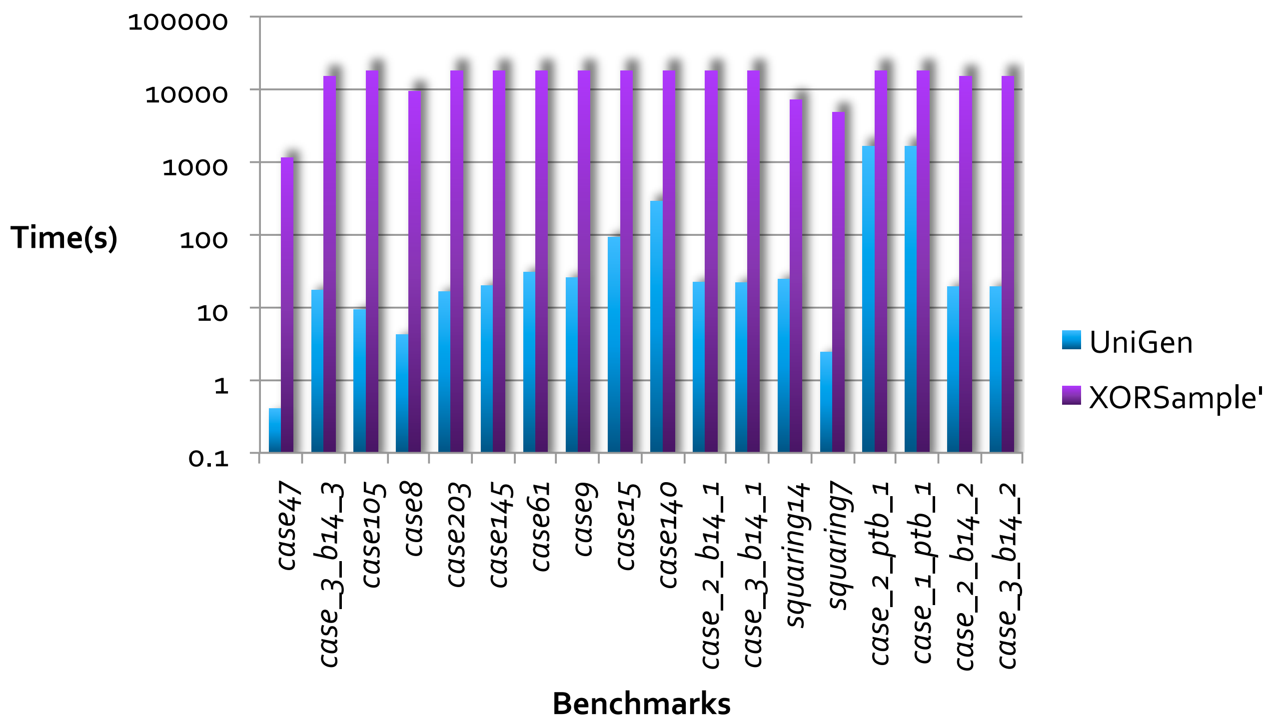
- Specialized for combinations of CNF and XORs
- Combine SAT solving with Gaussian elimination

UniGen Performance: Uniformity



Uniformity Comparison: UniGen vs Uniform Sampler

UniGen Performance: Runtime



Runtime Comparison: UniGen vs XORSample'

From Sampling to Counting

- Input formula: φ; Solution space: $Sol(\varphi)$
- **#SAT Problem**: Compute $|Sol(\varphi)|$
  - $\varphi = (p \vee q)$
  - $Sol(\varphi) = \{(0,1),(1,0),(1,1)\}$
  - $|Sol(\varphi)| = 3$

Fact: $\#SAT$ is complete for $\#P$ – the class of counting problems for decision problems in NP [Valiant, 1979].

Constrained Counting

A wide range of applications!

- Coverage in random-constrained verification
- Bayesian inference
- Planning with uncertainty
- ...

But: $\#SAT$ is really a hard problem! In practice, quite harder than SAT.

Approximate Counting

Trustworthy Approximation – **Probably Approximately Correct** (PAC):

- *Formula*: φ, *Tolerance*: ε, *Confidence*: $0 < \delta < 1$
- $|Sol(\varphi)| = \kappa$
- $Prob[\frac{\kappa}{(1+\varepsilon)} \leq \text{Count} \leq \kappa \times (1+\varepsilon) \geq \delta$
- Introduced in [Stockmeyer, 1983]
- [Jerrum+Sinclair+Valiant, 1989]: BPP^{NP}
- No implementation so far.

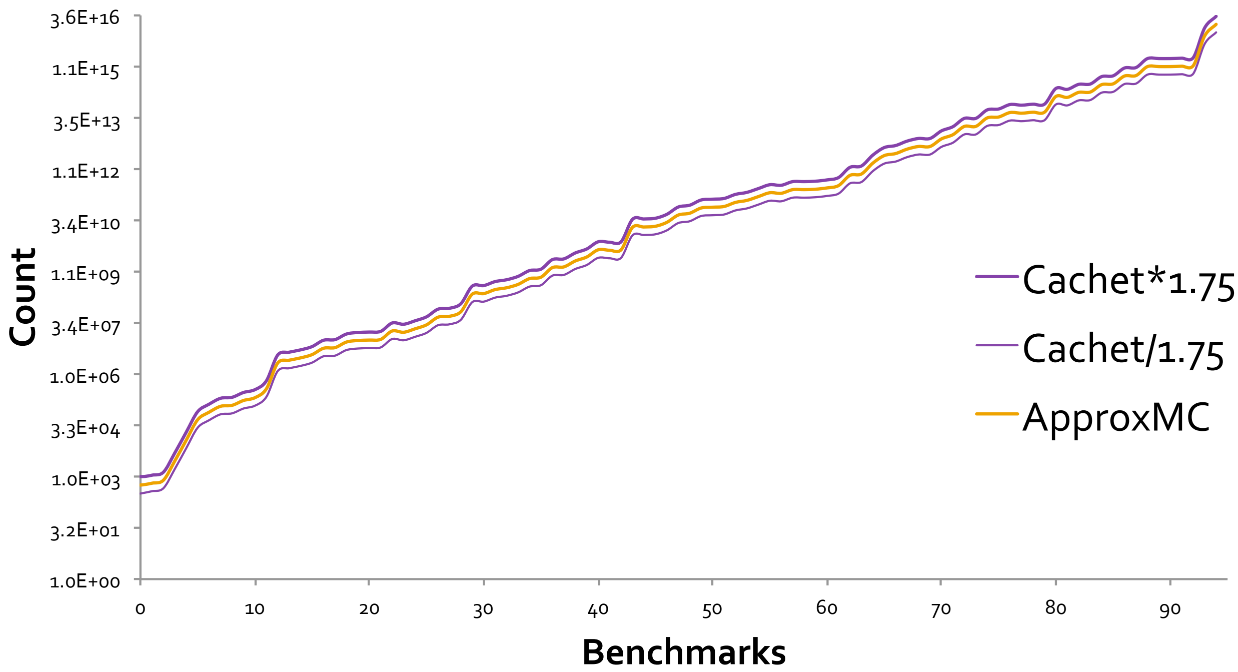
From Sampling to Counting

ApproxMC: [Chakraborty+Meel+V., 2013]

- Use m random XOR clauses to select at random an appropriately small cell.
- Count number of solutions in cell and multiply by 2^m to obtain estimate of $|Sol(\varphi)|$.
- Iterate until desired confidence is achieved.

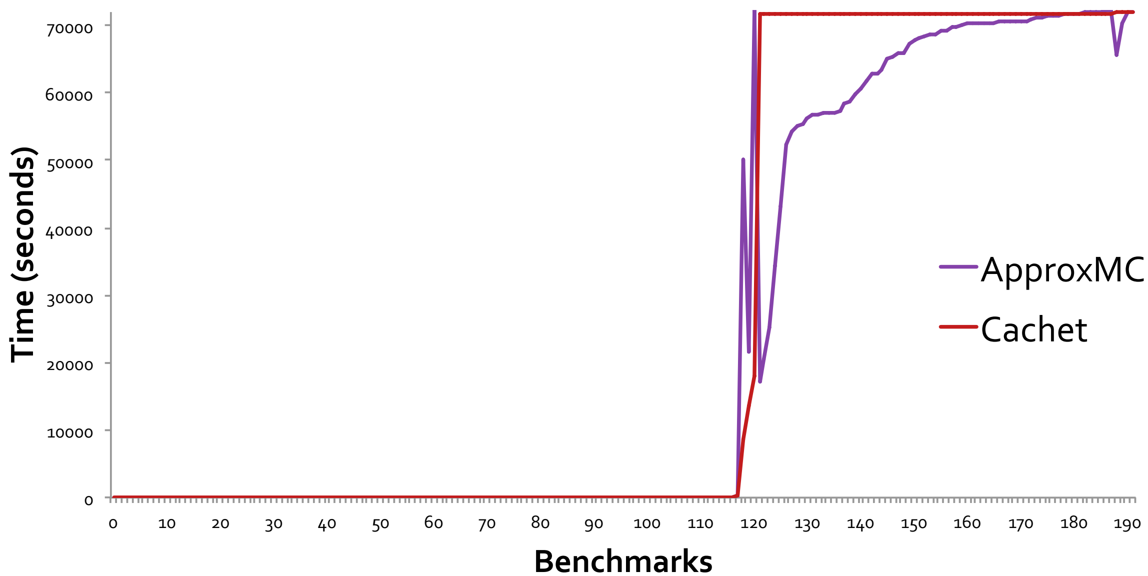
ApproxMC runs in time polynomial in $|\varphi|$, ε^{-1}, and $\log(1-\delta)^{-1}$, relative to SAT oracle.

ApproxMC Performance: Accuracy



Accuracy: ApproxMC vs Cachet (exact counter)

ApproxMC Performance: Runtime



Runtime Comparison: ApproxMC vs Cachet'

Back to Neural Nets

Baluta-Shen-Shinde-Meel-Saxena, CCS'19: *Quantitative Verification of Neural Networks And Its Security Applications*

Problem: Given a set N of neural networks and a property P of interest, defined over the union of inputs and outputs of neural networks in N , estimate how often P is satisfied.

Security Applications: robustness, Trojan attacks, fairness, etc.

Key Technology: ApproxMC!

SAT Solving

- The improvement in the performance of SAT solvers over the past 25 years is *revolutionary*!
  - Better marketing: Deep Solving
- SAT solving is an enabler, e.g., approximate sampling and counting
- When you have a big hammer, look for nails!!!
- Scalability is an ongoing challenge!

Reflection on P vs. NP

Old Cliché "What is the difference between theory and practice? In theory, they are not that different, but in practice, they are quite different."

P vs. NP in practice:

- P=NP: Conceivably, NP-complete problems can be solved in polynomial time, but the polynomial is $n^{1,000}$ – *impractical*!
- P≠NP: Conceivably, NP-complete problems can be solved by $n^{\log\log\log n}$ operations – *practical*!

Conclusion: No guarantee that solving P vs. NP would yield practical benefits.

Are NP-Complete Problems Really Hard?

- When I was a graduate student, SAT was a “scary” problem, not to be touched with a 10-foot pole.
- Indeed, there are SAT instances with a few hundred variables that cannot be solved by any extant SAT solver.
- But today’s SAT solvers, which enjoy wide industrial usage, routinely solve real-life SAT instances with millions of variables!

Conclusion We need a richer and broader complexity theory, a theory that would explain both the difficulty and the easiness of problems like SAT.

Question: Now that SAT is “easy” in practice, how can we leverage that?

- We showed how to leverage for sampling and counting. What else?
- Is BPP^{NP} the “new” $PTIME$?

From Model-Driven Computer Science to Data-Driven Computer Science and Back

In Summary:

- It is a *paradigm glide*, not *paradigm shift*.
- Data-driven CS *refines* model-driven CS, it does *not* replace it.
- Physicists still teach Mechanics, Electromagnetism, and Optics.
- But we must bridge the gap between machine learning and logic to get *human-centered AI*.