Quantitative Automated Reasoning: The Quest for Scalability

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Computing: The Story of an Endless Quest for Scalability Watson, 1940s: "I think there is a world market for about five computers." Gates & Allen, 1970s: "A computer on every desk and in every home" 2020: 22 billion IoT connected devices







satisfies







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Central Question Is it always the case that $\mathcal{M} \models \mathcal{P}$? Equivalently, can it be the case that $\mathcal{M} \land \neg \mathcal{P}$?



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Boolean Satisfiability (SAT): Given a Boolean formula, is there a solution, i.e., an assignment of 0's and 1's to the variables that makes the formula equal 1?

Example: $(X_1 \lor \neg X_2 \lor \neg X_3) \land (X_2 \lor \neg X_3)$ $X_1 = 1, X_2 = 1, X_3 = 1$



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[Circa 2012]: Now that SAT is "easy", it is time to look beyond satisfiability

Beyond SAT I: Quantification

PC2 (dbar[] SP, char[] UU) {
 math = true;
 for { int i=0; i<U1.isg(t); i++) {
 if (SP[i] = U[[i]) math=false;
 else math = math;
 if math return Yes;
 else return No;
 }
</pre>

Information Leakage



Fairness



Quantum Simulation



Critical Infrastructure

Beyond SAT I: Quantification

PC2 (char[] SP, char[] UD) {
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Quantification: How often does \mathcal{M} satisfy \mathcal{P} ?

Counting

Beyond SAT II: Reasoning about Distributions



- Multiple application domains require reasoning about distributions
- Constraints define the structure of relevant input spaces
- Challenge: How to efficiently sample from and analyze these distributions?

Beyond SAT III: Automated Synthesis



Synthesis

Beyond SAT III: Automated Synthesis



Synthesis

Beyond SAT III: Automated Synthesis



Synthesis



Research Overview



Artificial Intelligence AAAI:25×, IJCAI:13×, NeurIPS: 6×, KR:2×

Formal Methods/Constraints

Logic/Databases

PODS:7×, LICS:2×, LPAR:4×,

Software Engineering

ICSE:2 \times , FSE: 2 \times , CCS:1 \times

CAV:11×, SAT:10×, CP:9×, TACAS: 3×, DAC: 3×, ICCAD: 2×, DATE

Research Program's Output

Recent Research Paper Recognition

- Best/Distinguished Paper Awards: CAV-23, CAV-24, and ICLP-24
- Best Paper Award Nomination: ICCAD-22 and DATE-23
- Research Highlights: CACM (2023), ACM SIGMOD (2022)
- Knuth's Article on Distinct Elements (and media coverage)

Job Placement Highlights

- Teodora Baluta (PhD) \rightarrow Assistant Professor, Georgia Tech
- Priyanka Golia (PhD) \rightarrow Assistant Professor, CISPA (and IIT Delhi, India) ACM India Doctoral Dissertation Award 2024
- Tim van Bremen (post-doc) \rightarrow Assistant Professor, NTU Singapore
- Anna Latour (post-doc) \rightarrow Assistant Professor, TU Delft
- Gunjan Kumar (post-doc) \rightarrow Assistant Professor, IIT Kanpur
- Lawqueen Kanesh (post-doc) \rightarrow Assistant Professor, IIT Jodhpur
- Yong Lai (post-doc) → Associate Professor, Jilin University

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Today's Focus: Counting

Counting

- Given: A Boolean formula F over $X_1, X_2, \cdots X_n$
- Sol(F) = { solutions of F }
- SAT: Determine if Sol(F) is non-empty
- Counting: Determine |Sol(F)|

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- Generalization to arbitrary weights
 - Given weight function (implicitly represented) $W: \{0,1\}^n \mapsto [0,1]$
 - $W(F) = \sum_{y \in Sol(F)} W(y)$
 - (Weighted) Counting: Determine W(F)

Today's talk: We focus on unweighted case, i.e., |Sol(F)|

Today's Menu

Appetizer Applications

- Critical Infrastructure Resilience
- Quantitative Verification of AI Systems
- Quantum Simulation

Main Course ApproxMC: A Scalable Counting Framework

Dessert Future Outlook

Resilience of Critical Infrastructure Networks

[DMPV17,PDMV19, KM23]



Can we predict the likelihood of a blackout due to natural disaster?

Resilience of Critical Infrastructure Networks



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- G = (V, E); set of source nodes S and terminal node t
- failure probability $g: E \rightarrow [0, 1]$
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Constrained Counting

Key Idea: Encode disconnectedness using constraints

Impact: The first theoretically sound estimates of resilience in power transmission networks of ten medium sized cities in US

Our Focus: Binarized Neural Networks



Robustness Quantification

$$\left| \{ x : \mathcal{N}(x + \varepsilon) \neq \mathcal{N}(x) \} \right|$$

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Encode Symbolically

Constrained Counting

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Robustness Quantification

Fairness Quantification

 $\{x: \mathcal{N}(x+\varepsilon) \neq \mathcal{N}(x)\}$

Encode Symbolically

 $\{x : \mathcal{N}(x \land \text{Black}) \neq \mathcal{N}(x \land \text{White})\}$

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Constrained Counting

Impact: The first scalable technique for rigorous and certified quantification of robustness and fairness of Binarized Neural Networks

Quantum Circuit Simulation via Model Counting

[MBL24]



- Quantum state: superposition of 2^n basis states with amplitudes α_i
- Measurement collapses to classical state with probability $|\alpha_i|^2$
- Challenge: Exponential state space makes simulation intractable

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 - Boolean formula F encodes valid computation paths
 - Weight function W encodes quantum amplitudes
- Pr[measuring outcome x] = $|W(F \land outcome = x)|^2$

Impact: State of the art approach for large classes of circuits, enabling verification of quantum algorithms on classical hardware

Applications across Computer Science



Impact: Counting-based approach is now the state of the art for all these applications

So Fundamental Yet So Hard

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Stockmeyer, 1983: Probably Approximately Correct (PAC) aka (ε, δ)-guarantees

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• Not practical

SAT Solver \neq SAT Oracle

Performance of state of the art SAT solvers depends on the formulas

Snapshot from 2012

Scalability					
			 <u> </u>		\rightarrow

Theoretical Guarantees

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Theoretical Guarantees

State of the art tool in 2012 could handle one out of 1076 robustness instances

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How many people in Singapore like coffee?

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 - Potentially 2ⁿ queries

Can we do with lesser # of SAT queries – $\mathcal{O}(n)$ or $\mathcal{O}(\log n)$?

As Simple as Counting Dots



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As Simple as Counting Dots

Pick a random cell



Estimate = Number of solutions in a cell \times Number of cells

Challenge 1 How to partition into roughly equal small cells of solutions without knowing the distribution of solutions?

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- Designing function h: assignments \rightarrow cells (hashing)
- Deterministic *h* unlikely to work
- Choose h randomly from a large family H of hash functions

2-wise Independent Hashing

[CW77]

2-wise Independent Hash Functions

- To construct $h: \{0,1\}^n \to \{0,1\}^m$, choose m random XORs
- Pick every X_i with prob. $\frac{1}{2}$ and XOR them
 - $X_1 \oplus X_3 \oplus X_6 \cdots \oplus X_{n-2}$

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 - $X_1 \oplus X_3 \oplus X_6 \cdots \oplus X_{n-2}$
- To choose $\alpha \in \{0,1\}^m$, set every XOR equation to 0 or 1 randomly

$$X_1 \oplus X_3 \oplus X_6 \cdots \oplus X_{n-2} = 0 \tag{Q_1}$$

$$X_2 \oplus X_5 \oplus X_6 \cdots \oplus X_{n-1} = 1 \qquad (Q_2)$$

$$(\cdots)$$

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• Solutions in a cell: $F \land Q_1 \cdots \land Q_m$

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Random XOR-based Hash Functions

[CW77]

- A cell is small if it has $\approx \text{thresh} = 5(1 + \frac{1}{\epsilon})^2$ solutions
- Many solutions \implies Many cells & Fewer solutions \implies Fewer cells

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ApproxMC makes $O(\frac{1}{\epsilon^2} \cdot \log \frac{1}{\delta} \cdot \log n)$ SAT queries.

Handle reasonable formulas: reasonable grids, reasonable programs

2019: CP-13 paper selected as one of the 25 papers across 25 years of CP conference

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B. Cook: Virtuous cycle: application areas drives more investment in foundational tools, while improvements in the foundational tools drive further applications. Around and around.

The definition of "reasonable" changes after every iteration of the cycle

Closing Slide from Seminar at NUS in Feb 2017



2025 Target: $100 \times$ speedup over 2016



All experiments on the same hardware



All experiments on the same hardware



1896 instances from diverse applications All experiments on the same hardware

2016 630 instances, each in \leq 5000 seconds

2024 1291 instances, each in \leq 1 second



A speedup of $100,000 \times$ over 2016
ApproxMC: In Pursuit of Scalability



In Pursuit of Scalability

Sparse hashing Phase Transition Theoretical SAT-20 IJCAI-16,17,19 CP-19 CP-18, IJCAI-19 Advances LICS-20 PODS-21,22 CP-20 Chain Formulas Prob. Caching Algorithmic Constraints-16 IJCAI-15 TACAS-20, AAAI-21 IJCAI-19 Engineering ICCAD-22, DAC-24 NeurIPS-20, SAT-25 AAAI-23, CAV-25 Pseudo-Boolean **CNF-XOR** MaxSAT-XOR Hardware Accelerator Software CP-21 AAAI-19 KR-21 SAT-21 Development AAAI-24, AAAI-25 CAV-20, CAV-24 SAT-25

In Pursuit of Scalability



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SAT Solvers != SAT oracles

Modern SAT Solvers: Conflict-Driven Clause Learning (CDCL) paradigm

- Guess an assignment to subset of variables, if conflict, remember the reason
- Continue until satisfiable/unsatisfiable

CDCL and XORs: Random XORs are hard for CDCL in theory and practice

• But there is a polynomial time procedure: Gauss-Jordan Elimination

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level 0 1 2	dec ×1 ×3 ×4	\rightarrow \rightarrow	prop x_5 $x_2, \neg x_5$

CDCL

Gauss-Jordan Elimination

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Incremental CDCL

Incremental Gauss-Jordan Elimination

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Incremental Gauss-Jordan Elimination

Engineering an efficient CDCL-GJE solver

[SM19; SGM20]

- Data-structures for efficient propagation and conflict analysis
- Supervised machine learning-guided heuristics

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✓ Challenge 1 Need to handle CNF-XOR formulas Software Development Specialized CDCL-GJE Solver with Data-Driven Heuristics SAT Solvers != SAT oracles: Performance degrades with increase in the size of XORs

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Software Development Specialized CDCL-GJE Solver with Data-Driven Heuristics

SAT Solvers != SAT oracles: Performance degrades with increase in the size of XORs

- Pick every X_i with prob. $\frac{1}{2}$ and XOR them
- Expected size of each XOR: $\frac{n}{2}$

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Challenge 2 Do we have really to pick **every** variable X_i with prob $\frac{1}{2}$?

- Not all variables are required to specify solution space of F
 - $F := X_3 \iff (X_1 \lor X_2)$
 - X_1 and X_2 uniquely determines rest of the variables (i.e., X_3)
- $\mathcal{I} \subseteq X$ is independent support if it suffices to determine the solution space
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- Typically \mathcal{I} is 1-2 orders of magnitude smaller than X

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- Approach I: log *n* hard calls to SAT solver via reduction to GMUS [IMMV15] Best Student Paper, CP15
- Approach II: n easy calls to SAT solver via Padoa's theorem [SM22; SM24]

Approach II + ApproxMC is up to $100 \times$ faster than Approach I + ApproxMC SAT Solvers \neq SAT Oracles

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✓ Challenge 1 Need to handle CNF-XOR formulas

Software Development Specialized CDCL-GJE Solver with Data-Driven Heuristics

SAT Solvers != SAT oracles: Performance degrades with increase in the size of XORs

- Pick every X_i with prob. $\frac{1}{2}$ and XOR them
- Expected size of each XOR: $\frac{n}{2}$

✓ Challenge 2 Do we have to really pick every variable X_i with prob $\frac{1}{2}$? Algorithmic Engineering Pick $X_i \in \mathcal{I}$

How to partition into roughly equal small cells of solutions without knowing the distribution of solutions?

2-wise Independent Hash Functions

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Challenge 3 Do we have to really pick every variable X_i with **prob** $\frac{1}{2}$?

- If we pick with prob $p < \frac{1}{2}$, then no guarantees of 2-wise independence
- Z_m : Number of solutions in a randomly chosen cell
- 2-wise independence $\implies \frac{Var[Z_m]}{E[Z_m]} \leq 1 \implies$ Concentration bounds

[MA20]

Open problem (2013-19): Sparse $(p < \frac{1}{2})$ XORs that work in theory and practice

[MA20]

Open problem (2013-19): Sparse $(p < \frac{1}{2})$ XORs that work in theory and practice

Theorem (Log-Sparse XORs suffice)

If we pick m-th XOR with $p_m = \frac{\log m}{m}$, we have $\frac{Var[Z_m]}{E[Z_m]} \le 1.1$ Improvement of p from $\frac{m/2}{m}$ to $\frac{\log m}{m}$

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$$\frac{\mathsf{Var}[Z_m]}{\mathsf{E}[Z_m]} \leq 1 + |\mathsf{Sol}(F)|^{-1} \cdot \sum_{\substack{\sigma_1 \in \mathsf{Sol}(F) \\ w = d(\sigma_1, \sigma_2)}} \sum_{\substack{\sigma_2 \in \mathsf{Sol}(F) \\ w = d(\sigma_1, \sigma_2)}}^{\approx \text{ collision probability}}$$

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$$\frac{\mathsf{Var}[Z_m]}{\mathsf{E}[Z_m]} \le 1 + |\mathsf{Sol}(F)|^{-1} \cdot \sum_{\sigma_1 \in \mathsf{Sol}(F)} \sum_{\substack{\sigma_2 \in \mathsf{Sol}(F) \\ w = d(\sigma_1, \sigma_2)}} \underbrace{\sim \mathsf{collision probability}}_{r(w, p_m)} \underbrace{\le 1 + \sum_{w=0}^n \binom{n}{w} r(w, p_m)}_{\mathsf{Earlier Attempts}}$$

[EGSS14,ZCSE16,AD17,ATD18]

[MA20]

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Rewrite
$$\sum_{\substack{\sigma_1 \in \mathsf{Sol}(F) \\ w = d(\sigma_1, \sigma_2)}} \sum_{\substack{r(w, p_m) = \sum_{w=0}^n C_F(w) r(w, p_m) \\ C_F(w) = |\{\sigma_1, \sigma_2 \in \mathsf{Sol}(F) \mid d(\sigma_1, \sigma_2) = w\}|}$$

Isopmerimetric Inequalities: Possible to bound $C_F(w)$ if bound on |Sol(F)| is known Barrier: But |Sol(F)| can be arbitrarily large

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Isopmerimetric Inequalities: Possible to bound $C_F(w)$ if bound on |Sol(F)| is known Barrier: But |Sol(F)| can be arbitrarily large Key Idea: In the context of Z_m , It suffices to assume $|Sol(F)| < 2^{m+u}$ for small u.

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✓ **Challenge 3** Do we have really to pick every variable X_i with **prob** $\frac{1}{2}$? **Theoretical Advances** Pick m-th XOR with $p_m = \frac{\log m}{m}$

In the Pursuit of Scalability



Reliability of Critical Infrastructure Networks



Timeout = 1000 seconds

Reliability of Critical Infrastructure Networks



Timeout = 1000 seconds

Reliability of Critical Infrastructure Networks



Timeout = 1000 seconds

Impact: The first theoretically sound estimates of resilience in power transmission networks of ten medium sized cities in US $\,$

ApproxMC: Progress over the years



1896 benchmarks from diverse applications

Time taken (seconds) for an instance 2016: 3552.16 2019: 32.83 2020: 19.59 2022: 0.15 2024: 0.02 A speedup of 100,000× over 2016

Another Iteration of Virtuous Cycle

B. Cook, 2022: Virtuous cycle: ...application areas drives more investment in foundational tools, while improvements in the foundational tools drive further applications. Around and around.

SharpTNI: Counting and Sampling Parsimonious Transmission Networks under a Weak Bottleneck Palak Sashital¹ and Mohammed ErKelir²¹

Check before You Change: Preventing Correlated Failures in Service Updates

Ennan Zhai[†], Ang Chen[‡], Ruzica Piskac[°], Mahesh Balakrishnan^{§,*} Bingchuan Tian[‡], Bo Song[•], Haoliang Zhang[•]

Automating the Development of Chosen Ciphertext Attacks

Gabrielle Beck, Maximilian Zinkus, and Matthew Green, Johns Hopkins University

Static Evaluation of Noninterference using Approximate Model Counting

Ziqiao Zhou Zhiyun Qian

Michael K. Reiter

Yingian Zhang

A Study of the Learnability of Relational Properties

Model Counting Meets Machine Learning (MCML)

Muhammad Usman	Wenxi Wang	Marko Vasic
University of Texas at Austin, USA	University of Texas at Austin, USA	University of Texas at Austin, USA
manammatasmangratexas.eou	werke up to exact the	vasceptizeration
Kaiyuan Wana"	Haris Vikalo	Sarfray Khurshid

Quantifying Software Reliability via Model-Counting

Samuel Teuber⁽¹⁸⁾[©] and Alexander Weigl[©]

IN SEARCH FOR A SAT-FRIENDLY BINARIZED NEU-RAL NETWORK ARCHITECTURE

Nina Narodytska

Hongce Zhang*

Quantifying the Efficacy of Logic Locking Methods

Joseph Sweeney, Deepali Garg, Lawrence Pileggi

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Model Counting Competition

MC-2024

Tracks Rodel Counting, Respired Nogel Counting, Negative Nodel Counting (Regative weights), Projected Model Counting, Property Negative Media Gaurding (Interpreter, Marchan Counting), Interla, Interland, and Park, advers, competition Instances, adverted Levalnes

MC-2623

 Trustes Blockel Counting, Weighted Model Counting, Projected Madel Counting, Projected Weighted Model Counting (Scontore, Starbace Counting, Some, wrees, receiv, Seco., Severa, competition reterrors, substatute terreterrors)

Part of FLaC Dys

 Trans. Model Counting, Mediated Model Counting, Protected Model Counting, Protected Weighted Model Counting MC-2021

Tracio: Hodel Counting, Weighted Model Counting, and Projected Model Counting

MC-2020

The results of each Model Counting Competition are documented in a report.

• Tracks Redet Counting, Weighted Road Counting, and Projected Model Counting documents, format, which, report, service, proved, Sorgerberg Header Counting, and the Sorgerberg Header Counting of the So

Workshops

 2021 Workshop on Gausting, Bangling, and Byshaels (in person even) constant 2023 Workshop on Causting and Bangling (in person even) Constant Constant, even Constant, even Volumity 2021 Volumity 2021

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Kaiyuan Wans"	Haris Vikalo	Sarfraz Khurshid

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Generalizability

Union of Sets ApproxMC is Fully Polynomial Randomized Approximation Scheme (FPRAS) – fundamentally different from the Monte-Carlo based FPRAS

- IJCAI-19 Sister Conferences Best Paper Award Track
 [MSV19]
- Praise by Donald Knuth and coverage in popular media (Quanta Magazine) [CVM22]

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Streaming Counting over a stream: Distinct Elements Example: How many unique customers visit website? Fundamental problem in Databases

• CACM 2023 Research Highlights

[PVBM21]

ACM SIGMOD 2022 Research Highlight

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- CACM 2023 Research Highlights
- ACM SIGMOD 2022 Research Highlight

[PVBM21]

Unsatisfiable Subsets Count minimal subsets of clauses that are unsatisfiable. Diagnosis metric for systems

ICLP-24 Best Paper Award

[K**M**24]

Counting, Sampling, and Synthesis



In Pursuit of Scalability



Figure: Counting over the years

In Pursuit of Scalability







ICCAD-21 & DATE-23 Best Paper Award Nomination

Where do we go from here?

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The Quest for Scalability is Endless

B. Cook, 2022: Virtuous cycle: ...application areas drives more investment in foundational tools, while improvements in the foundational tools drive further applications. Around and around.

Today's Quantitative Automated Reasoning tools

 \approx

Qualitative Reasoning tools (SAT/SMT) in early 2000s

Where do we go from here?

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Today's Quantitative Automated Reasoning tools

 \approx

Qualitative Reasoning tools (SAT/SMT) in early 2000s

The Time is Now

- LLMs enable rapid system creation \rightarrow Critical need for verification
- The achilees heel of formal methods adoption: formalization of complex systems
- LLMs excel at enabling rapid formalization of complex systems

This is the perfect time to do automated reasoning!

Industrial Practice: 100× Speedup

The Pursuit of Scalablity

Mission 2030: 100× Speedup for Quantitative Reasoning Tasks

Challenge Problems (for Counting)

Civil Engineering Rigorous resilience estimation for power grid of Los Angeles Al Safety Quantized neural network with 1M neurons Quantum Simulation Quantum Simultion for 1000 qubits.

Technical Directions (for Counting)

Theoretical Advances Native reasoning over expressive theories (*Beyond SMT*) Algorithmic Engineering Machine Learning-guided heuristic design Software Development Hardware-accelerator aware tools

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Certification: Approximate count is "correct" or the distribution generated is correct

- Applications to verification of probabilistic programming
- Building on recent advances in distribution testing
- Preliminary Work: AAAI-19, NeurIPS-20, NeurIPS-21, CP-22, NeurIPS-22, ICML-24, ICLR-25

It Takes a Village

Research Group

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Quantitative Automated Reasoning





These slides are available at https://www.cs.toronto.edu/~meel/talks.html

Detailed Future Directions

Applications: Infrastructure Resilience, Information Leakage, Prob. Databases, Configuration Testing, Partition Function, BNN Verification

Theoretical Advances Formula-based Sparse-XORs DNF, Minimal Solutions, Chain formula **Revisiting FPRAS** Permanent, Automata, Linear Extensions Parameterized Complexity Addition of XORs Streaming Delphic Sets Synthesis A theory of learning from relations **Entropy** Reduction in the number of gueries Algorithmic Engineering Incremental Incremental Counting Queries **Bit-vectors** Partitioning; Independent Support Heuristic ML-guided heuristic synthesis **Distributed** Streaming techniques SMT Synthesis SMT Formula Learning Beyond Qualititative Synthesis Optimal Functions, Approximate Synthesis Software Development Tighter Integration Multiple Queries Hybrid Constraints Callbacks XOR Handling PB-XOR, BNN-XOR, MaxSAT-XOR, ASP-XOR Accelerators GPU Knowledge Compilation SMT, Portfolio Certification **Distribution** Probabilistic Programming Equivalence **Counting** Certificate for Approximation