CSC 2547H: AUTOMATED REASONING WITH MACHINE LEARNING

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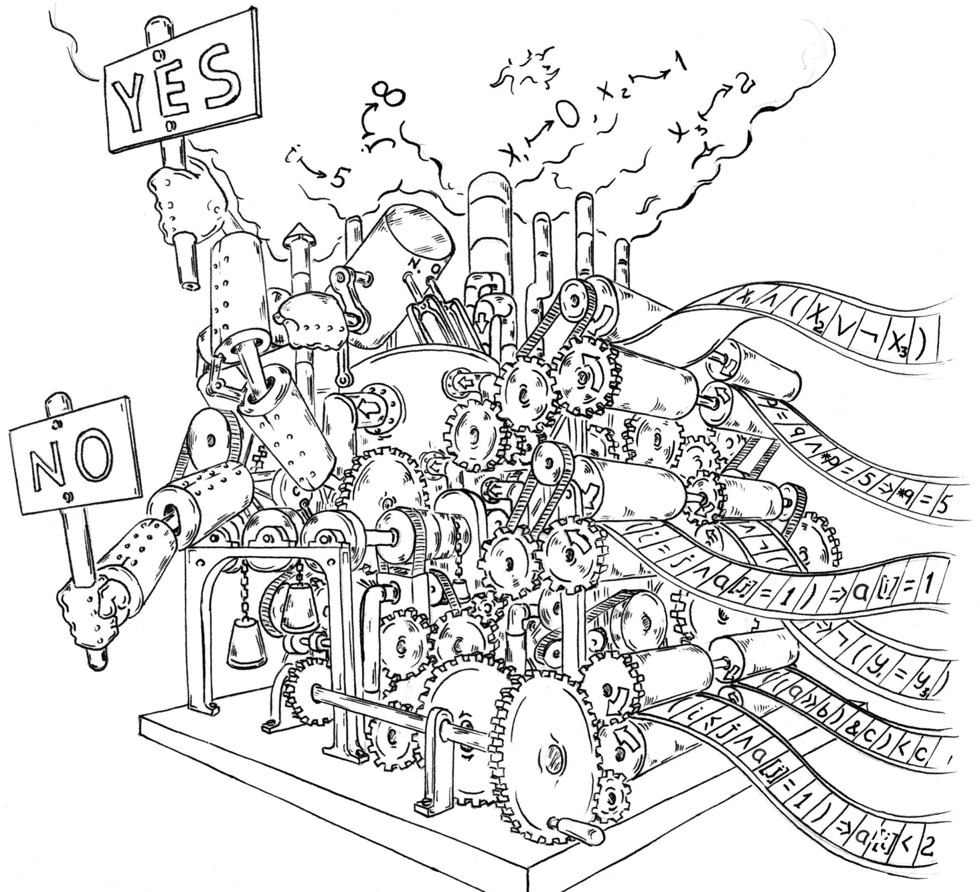
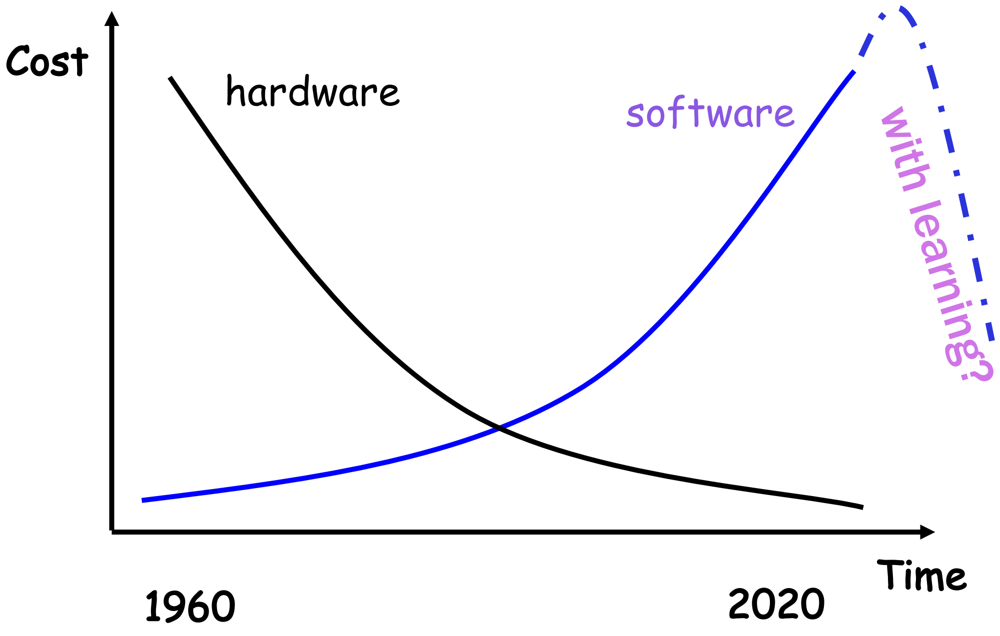


Course Overview

- **Goal**
  - Introduction to the cutting-edge research on *combining reasoning and machine learning*
  - Understand relevant *techniques* and learn to use the state-of-the-art *tools*
  - With a special focus on *symbolic constraints solving* and *programming applications*
- **Prerequisites**
  - CSC373H1 Algorithm Design, Analysis & Complexity
  - CSC324H1 Principles of Programming Languages
  - CSC311H1 Introduction to Machine Learning
- **Evaluation**
  - Class participation (10%): attendance, in-class/online discussions
  - One Assignment (15%): "solver-aided" programming
  - Paper presentation + QAs (15%): 15-minute presentation by every student
  - Project (proposal 15%, presentation 20%, report 25%): up to 4 students/group

Course Structure and Schedule

- **Week 1-3: Intro to reasoning challenges**
  - SAT (week 1), SMT (week 2), Program Analysis & Synthesis (week 3)
- **Week 4-10: Paper presentations (~8 per week)**
  - Week 4: Machine learning for SAT
  - Week 5: Machine learning for SMT
  - Week 6: Formal methods for machine learning
  - Week 7: Classic machine learning for code
  - Week 8: Deep learning for code
  - Week 9: Deep learning and logic programming
  - Week 10: Neuro-symbolic systems
- **Week 11-12: Project presentations**



Presentation guidelines

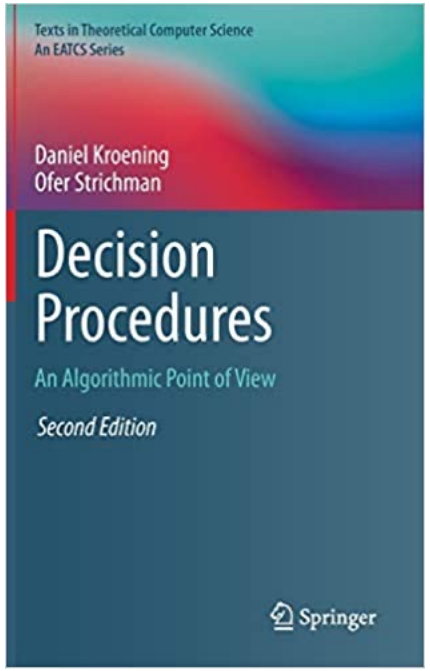
- **Preparation**
  - Start as early as possible (at least two weeks in advance)
    - Check the course schedule: https://www.cs.toronto.edu/~six/csc-2547hs-w23.html
    - Make a post on Ed and indicate which paper you would like to present
  - Meet TA and ask for feedback (at least one week in advance)
  - Prepare a video recording (before the class)
- **Content**
  - Background
  - Problem & challenges
  - Main idea
  - Main results + demo (bonus)
  - Related/future work
- **Tips**
  - Clarity is most important (an obscure and confusing presentation is meaningless)
  - Your main goal is to teach others something cool from the selected paper
  - A big plus is to inspire others and yourself through your presentation

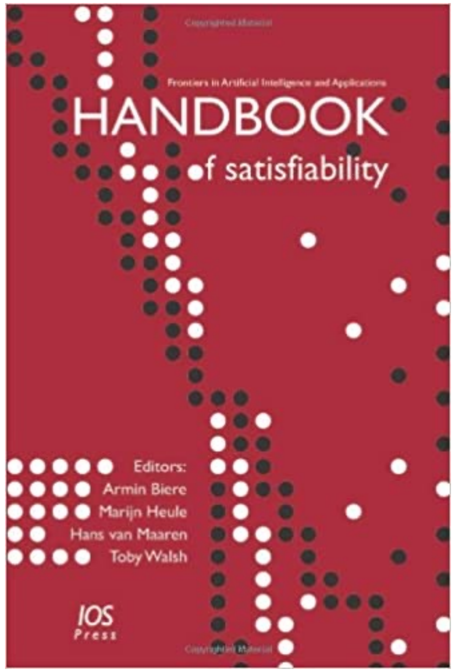
Logistics

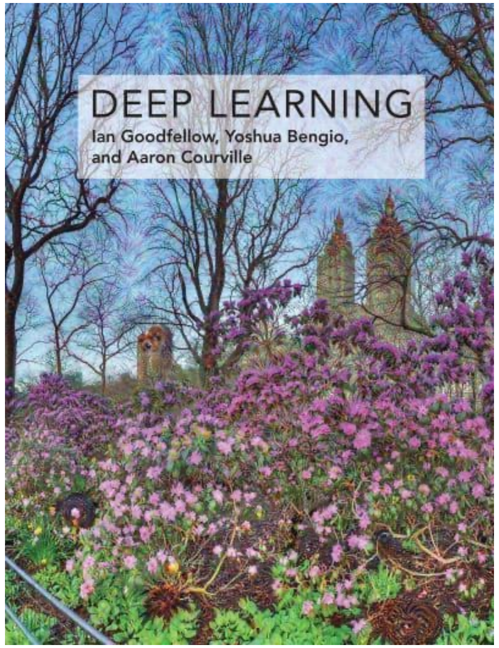
- **Office Hours**
  - Instructor, Tuesday, 3 PM – 4 PM, BA 7072
  - TAs, 2 hours/week
  - Or by appointment
- **Online Discussions**
  - Ed
  - Ideally, all questions should go to Ed. Your post can be private if needed.
- **Late submission policy**
  - 15% off / day
- **No plagiarism (absolutely)**
  - Plagiarism detection software will be used
- **No eating, drinking, etc. in class**

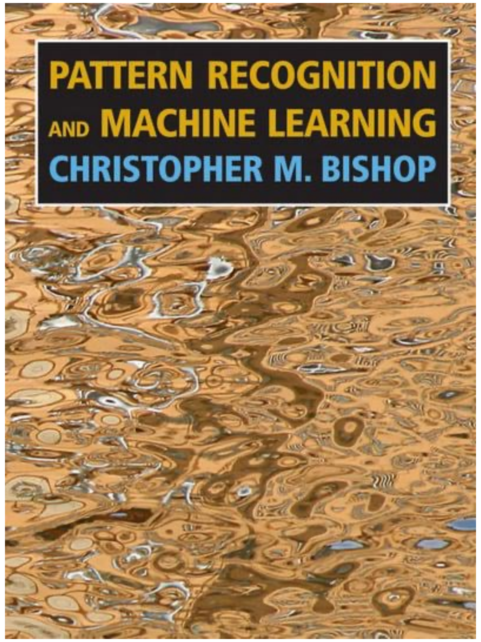
Supplemental Textbooks

- **No need to buy any**
  - Recommended by not required
  - You can find (free) online copies









Instructor and TAs

- **Instructor: Xujie Si**
  - Assistant Professor
    - UofT: 2023 – now
    - McGill/Mila: 2021–22
  - PhD from UPenn (2020)
  - Homepage: https://www.cs.toronto.edu/~six/index.html
- **Office: BA 7202**
- **Research interests:**
  - PL: Program analysis, synthesis & verification
  - AI: Symbolic constraint solving, deep learning, neuro-symbolic systems

Intro - Jonathan Lorraine

- 4th year PhD candidate in machine learning group
- Advised by David Duvenaud
- Did MScAC at U of T beforehand

- My research focuses on nested optimization in Machine Learning
  - Hyperparameter optimization, learning in games, amortized optimization, …

- Homepage for more: https://www.cs.toronto.edu/~lorraine/

TA Intro: Zhaoyu Li

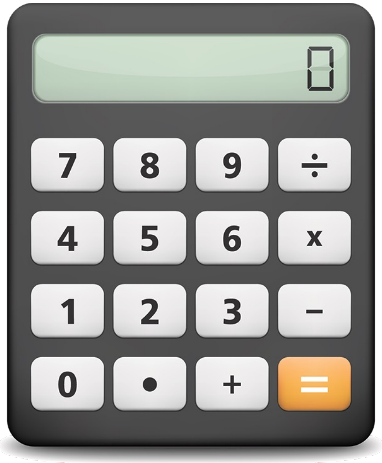
- **2nd year PhD student**
  - Spent 1st year at McGill / Mila
  - Bachelor degree from Shanghai Jiao Tong University
- **Research Interests**
  - Neuro-symbolic learning and reasoning
  - Automated theorem proving
- **Homepage**
  - https://www.zhaoyu-li.com/

Some caveats (before we have fun) …

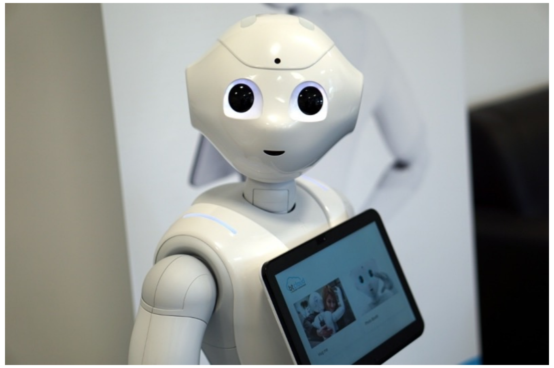
- **Lots of paper reading**
  - 60+ research papers (see the tentative schedule)
  - Most are quite technical (you are required to read at least one carefully and deeply)
- **Lots of “hacking” (in different languages)**
  - Hand-on experiences of using/building/analyzing solvers
  - Kind of data scientist + system programming experts
- **Some necessary skills/traits**
  - Strong desire to learn new things (no one can force you to learn if you don’t want to)
  - Don’t be afraid of exotic notations (they are just notations, the ideas behind are essential)
  - Understand things with unknowns
  - Learn to read quickly (by ignoring some details)
  - Learn to debug complicated systems (by abstracting away certain details)

What is intelligence?

Can compute fast?

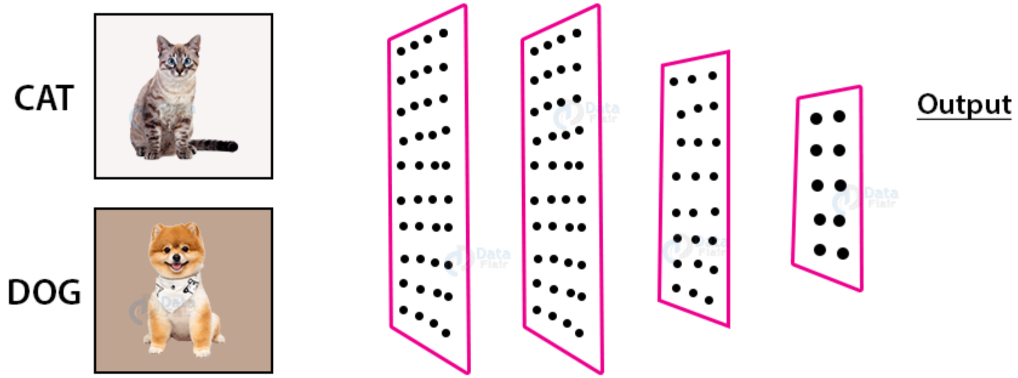


Look like human?



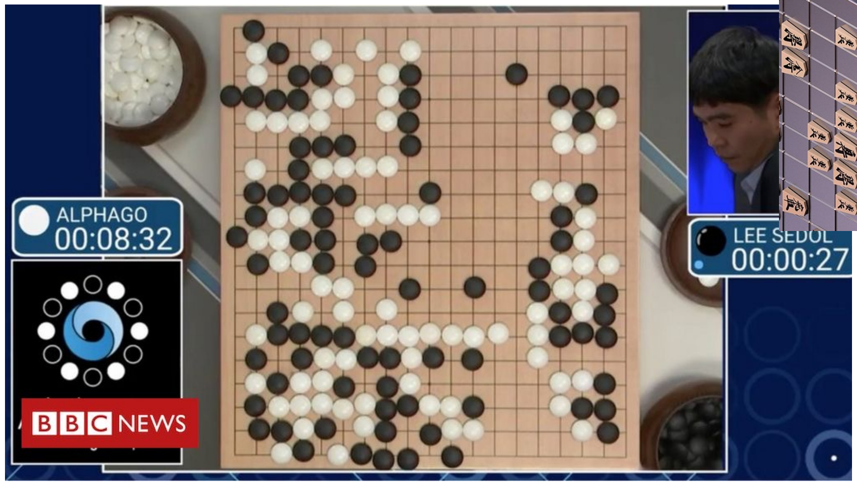
Compute faster?
fastest?

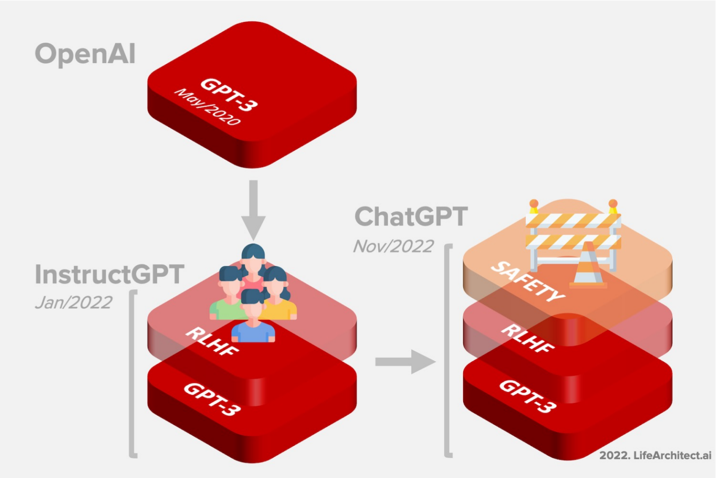
Can differentiate cats from dogs?



Can drive?

What is Intelligence? (Cont.)



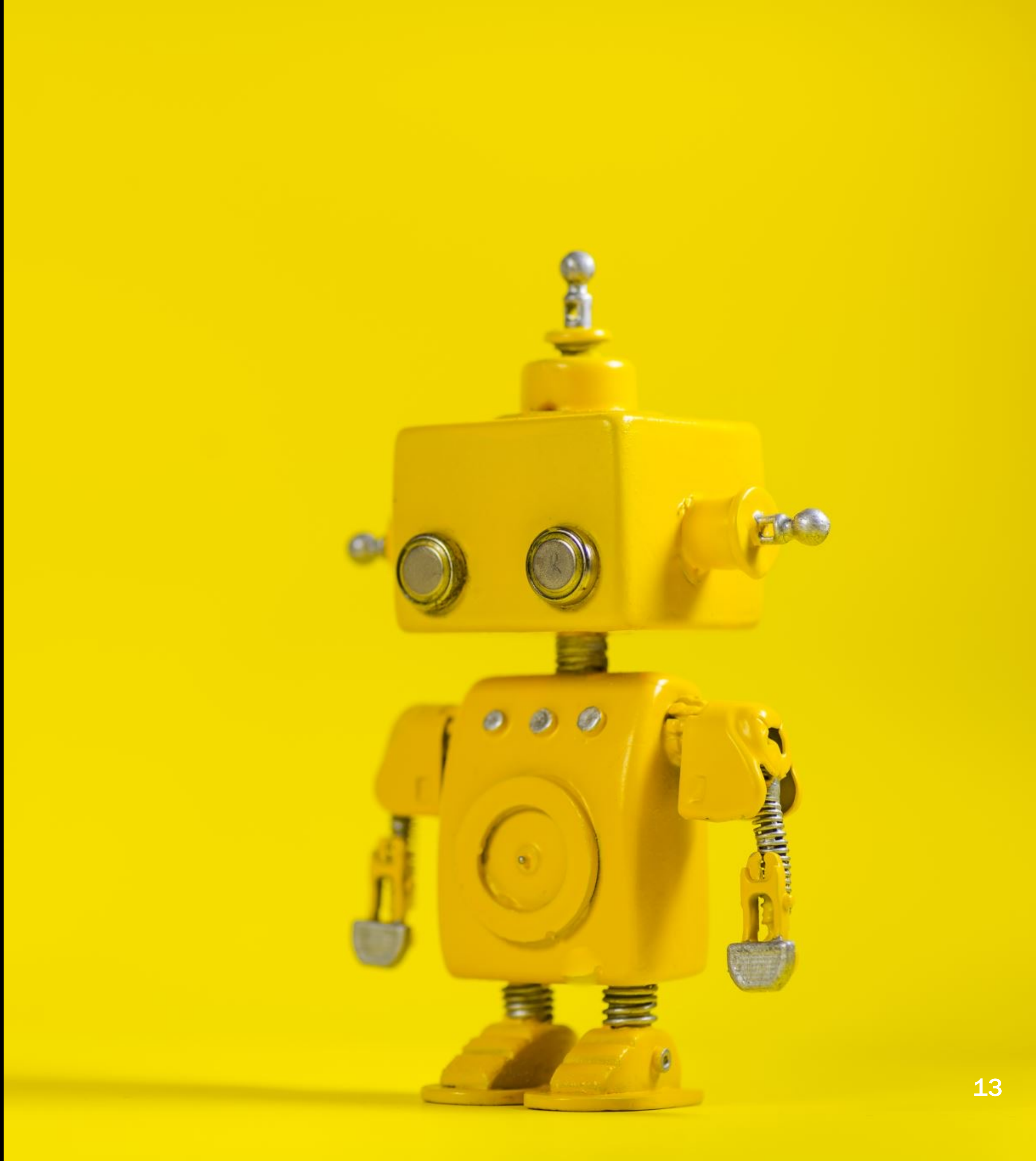


ARTIFICIAL GENERAL INTELLIGENCE

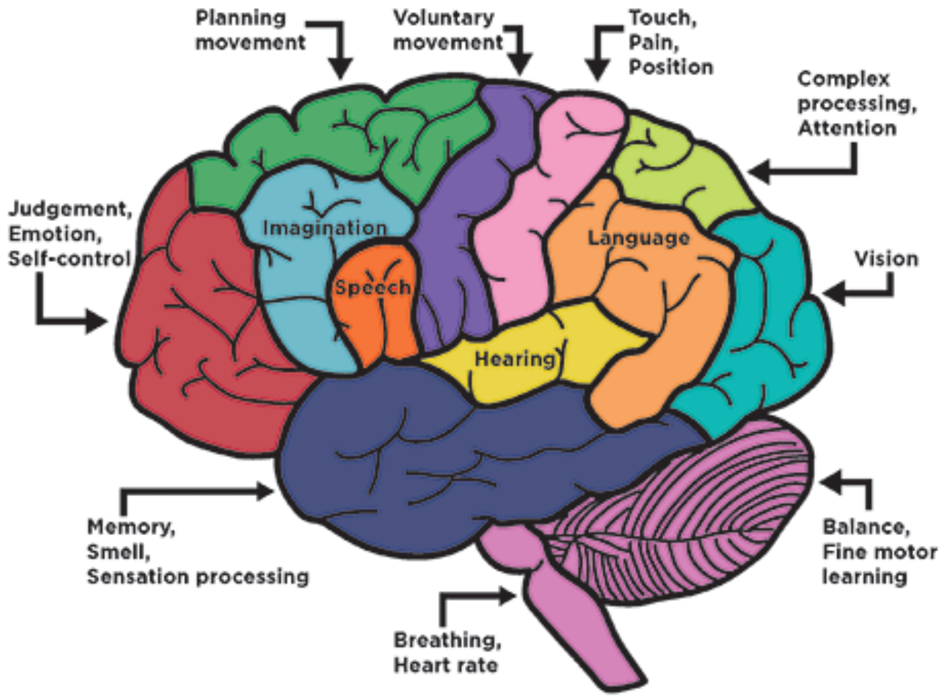
Human Intelligence, Animal Intelligence, Machine Intelligence, Alien Intelligence, you-name-it, ...

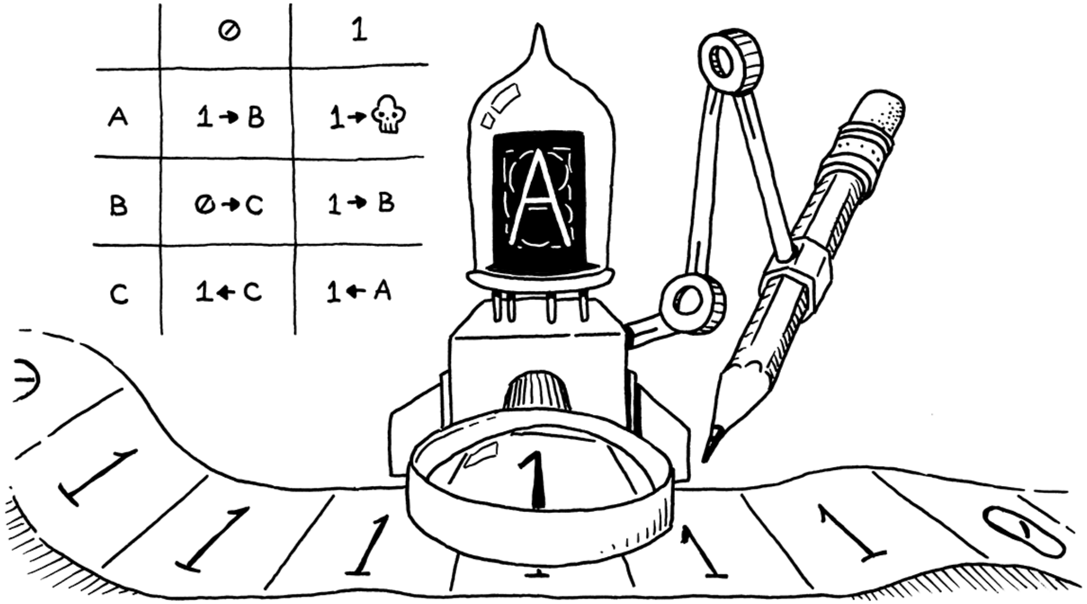
Which one is the strongest (so far)?

Which one will be the strongest?



Human Brain vs Turing Machine



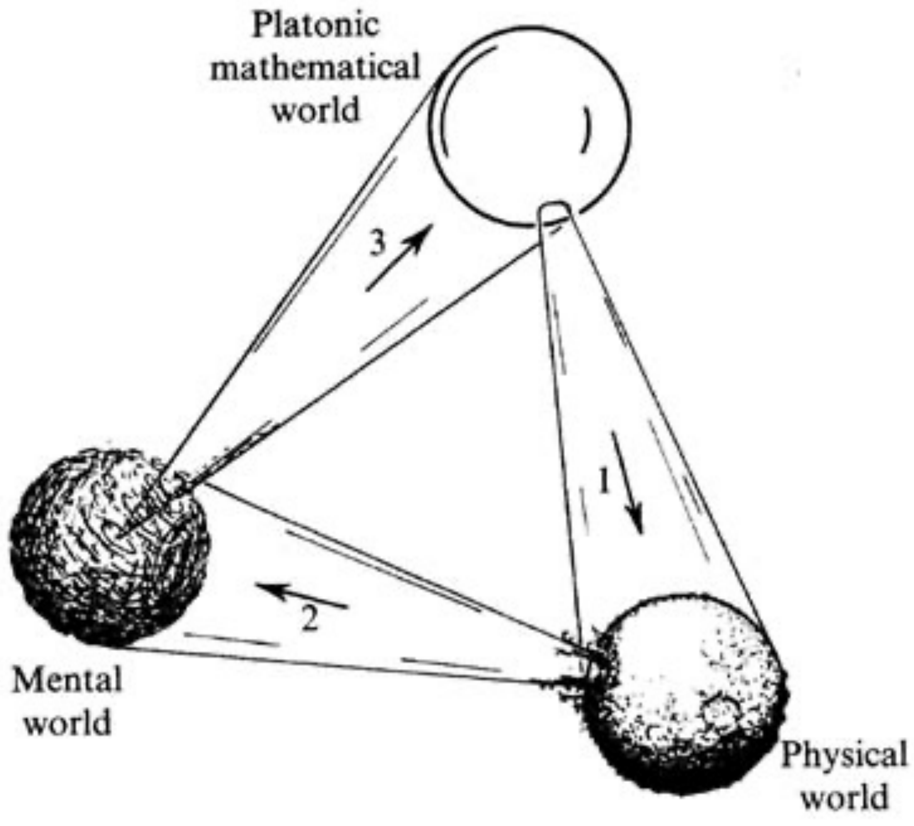


After billion years of evolution, the universe produces intelligent brains

No computers can be more powerful than a Universal Turing Machine

Penrose's three worlds philosophy

- Brain is fully determined by physics laws
- Physics laws are fully described by Math
- Math is created(?) by brain



Hardness Measure: NP-Complete, Undecidability

- **NP-complete (proudly originated from UofT)**
  - Nondeterministic Turing machine
  - Polynomial-time complete
  - A solution can be checked in polynomial time (on a deterministic Turing machine)
  - 3-SAT is the first well-known NP-complete problem (Cook, 1971)
- **Undecidability**
  - Impossible to construct an algorithm that always leads to yes-or-no answer
  - Regardless how long the algorithm may return
  - Halting problem is the first well-known undecidable problem

Main Progress: Heuristics + Engineering

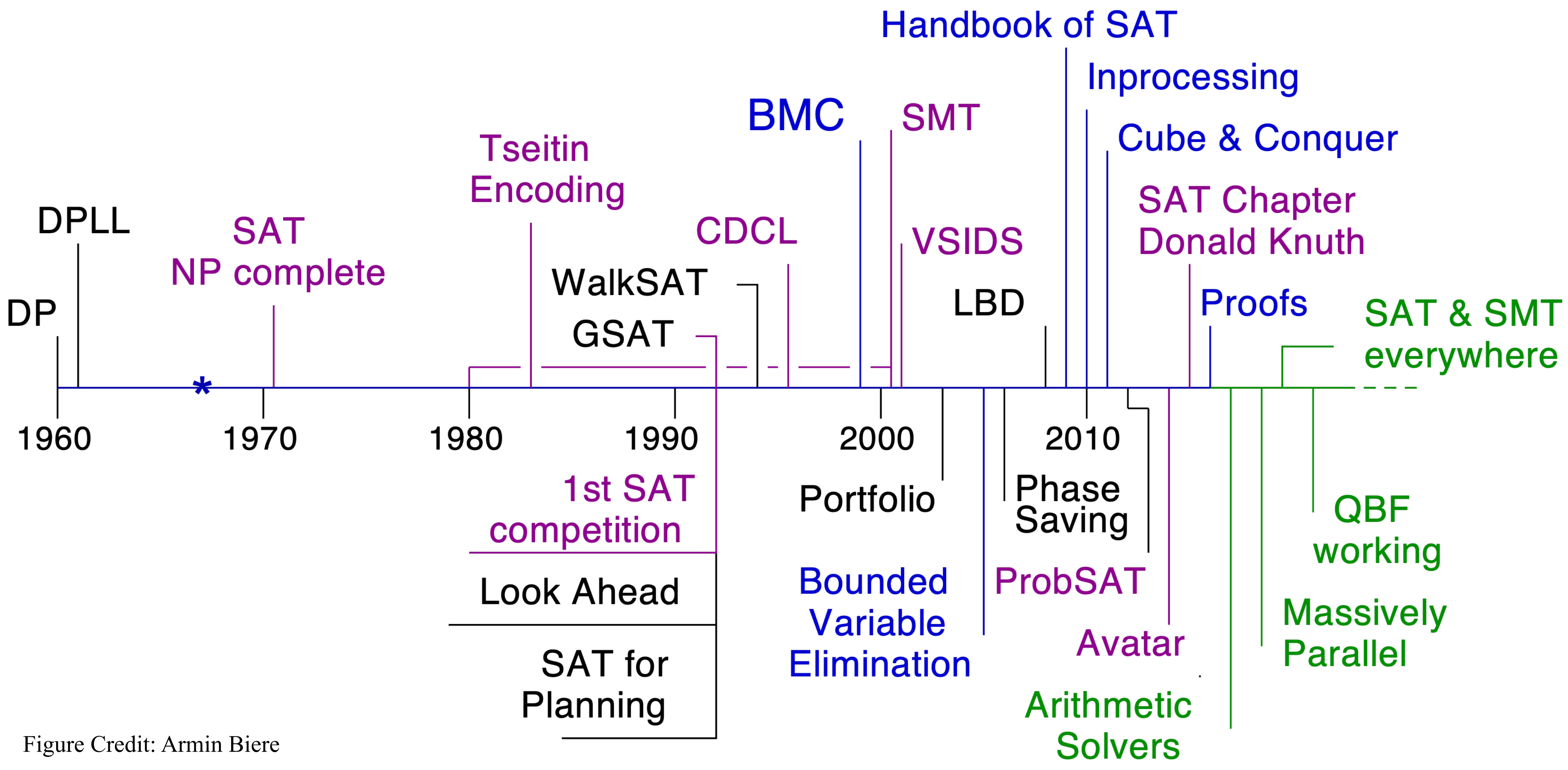
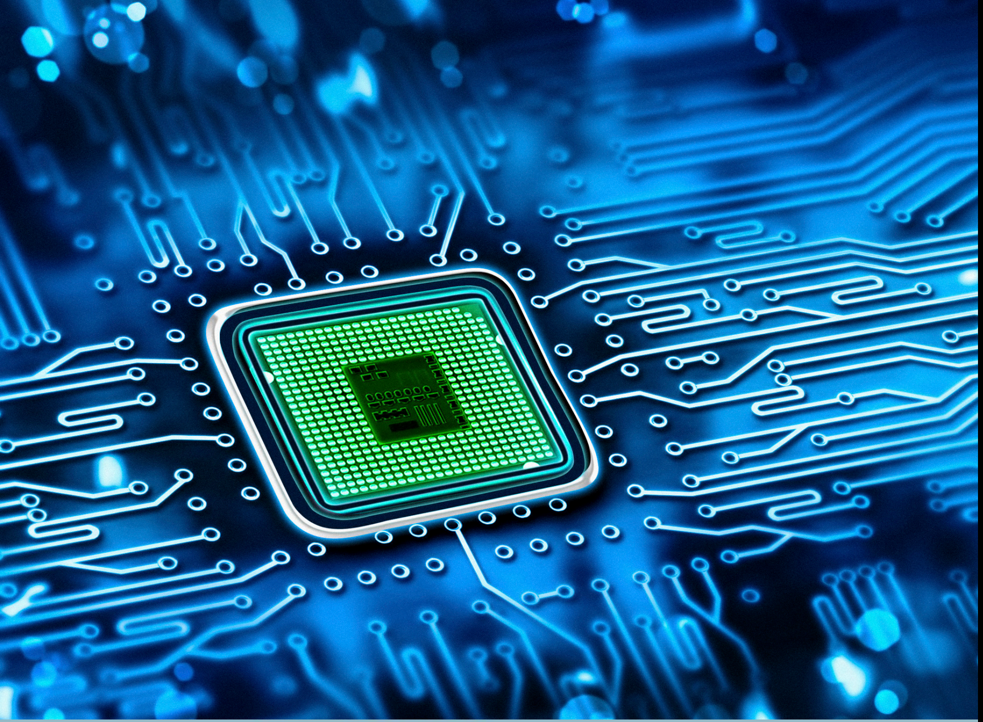
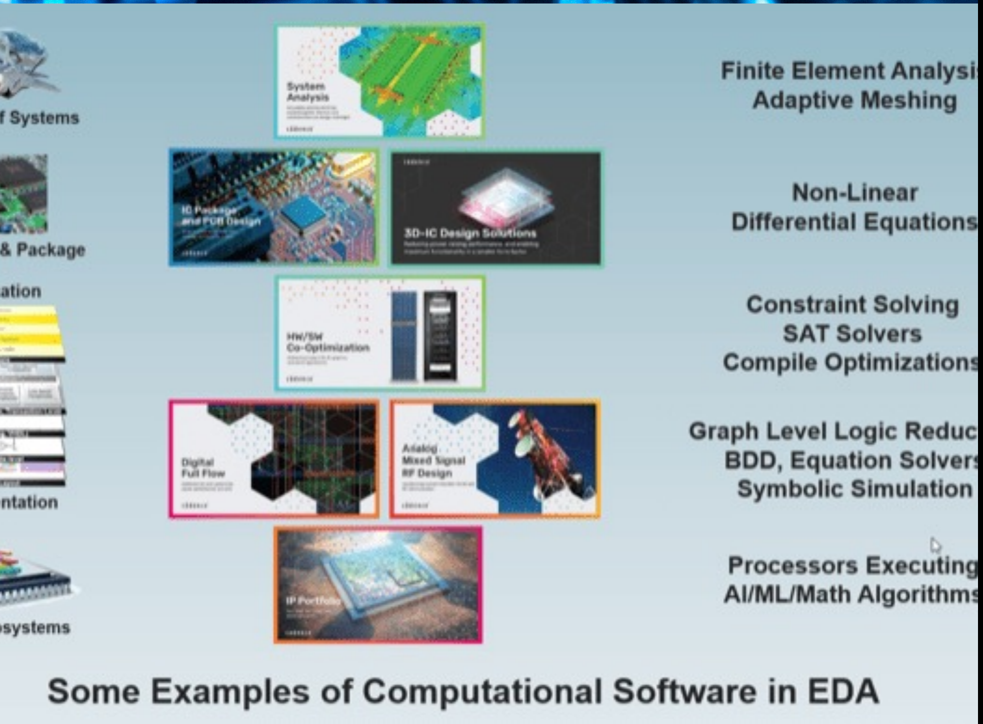


Figure Credit: Armin Biere

WHY DOES IT MATTER?





IMPORTANT APPLICATIONS IN EDA

A problem has been detected and Windows has been shut down to prevent damage
to your computer.

UNMOUNTABLE_BOOT_VOLUME

If this is the first time you've seen this error screen,
restart your computer. If this screen appears again, follow
these steps:

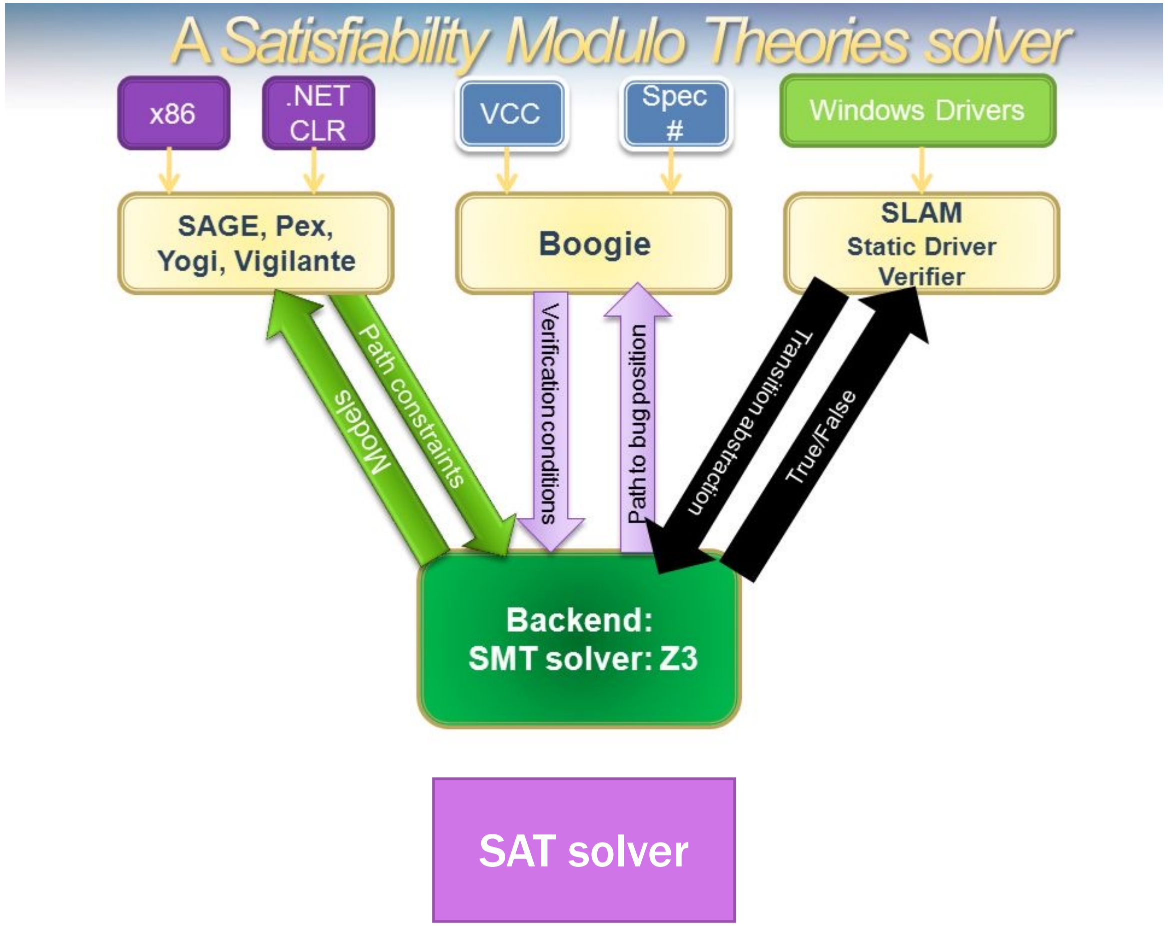
Check to make sure any new hardware or software is properly installed.
If this is a new installation, ask your hardware or software manufacturer
for any Windows updates you might need.

If problems continue, disable or remove any newly installed hardware
or software. Disable BIOS memory options such as caching or shadowing.
If you need to use Safe Mode to remove or disable components, restart
your computer, press F8 to select Advanced Startup Options, and then
select Safe Mode.

Technical Information:

*** STOP: 0x000000ED (0x80F128D0, 0xc000009c, 0x00000000, 0x00000000)

A Killer Application: Software Verification



NOT JUST WINDOWS...

Shortly after the first successful moon landing, Dijkstra spoke to the head of development for the module software:

"How did you produce so many lines of perfect code?"

"Huh? We had a bug a few days before launch, it accidentally calculated the moon as repelling rather than attracting."

"Wow! Those guys were lucky to make it alive, then!"

Cannot be always lucky ...

Got a speeding ticket??
It is kilometer NOT mile!!

Information Technology

Verification Tools Secure Online Shopping, Banking

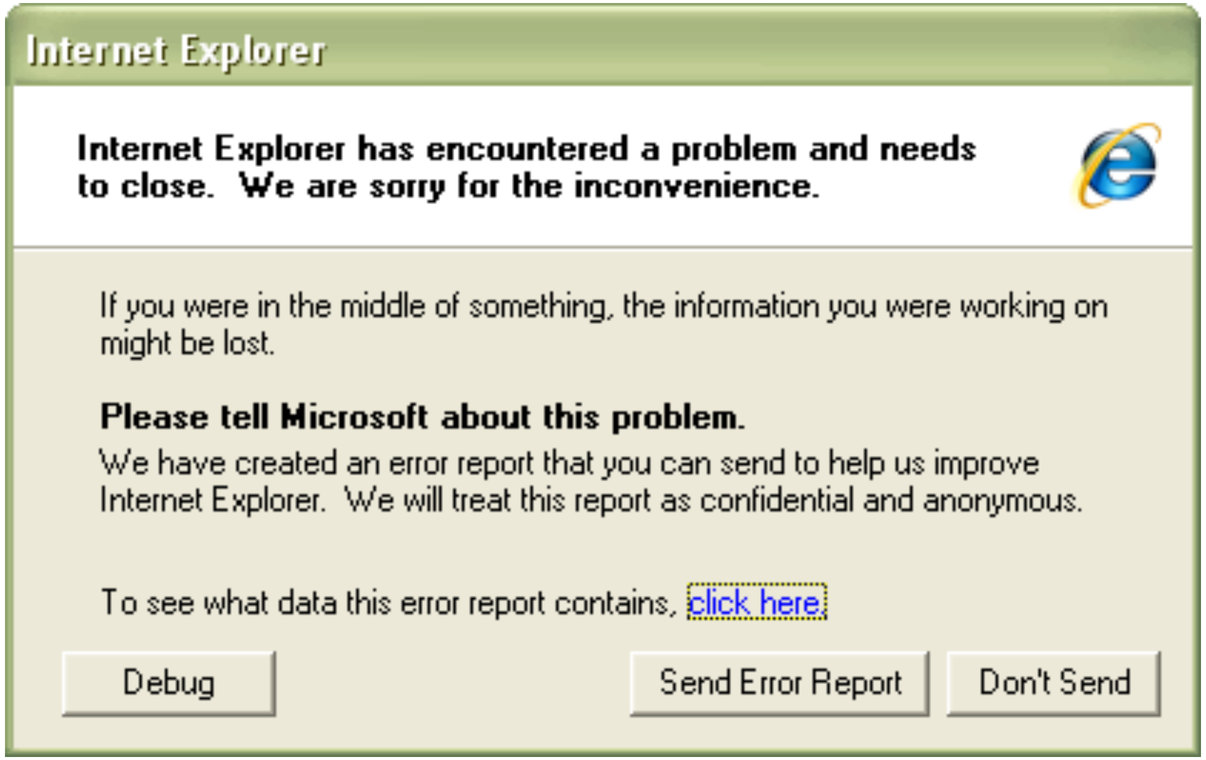
Originally published in 2010

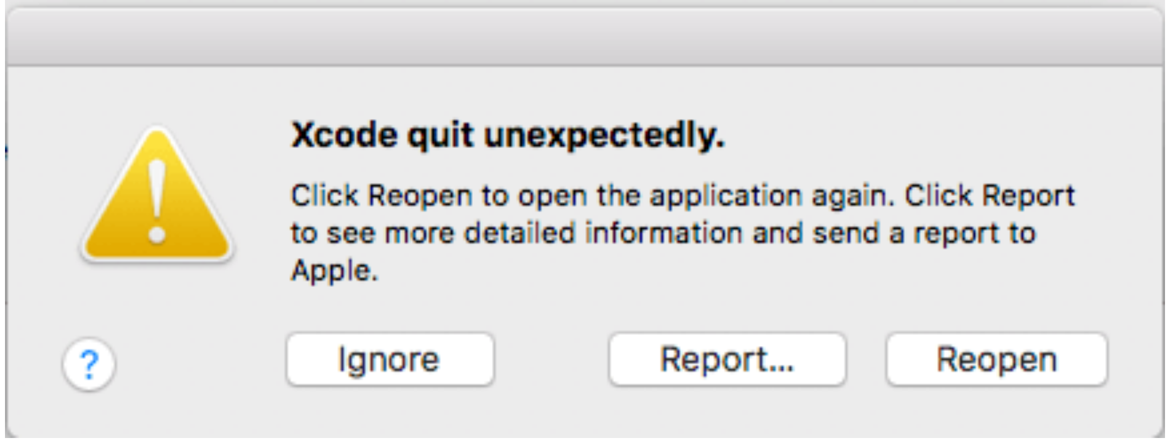
Originating Technology/NASA Contribution

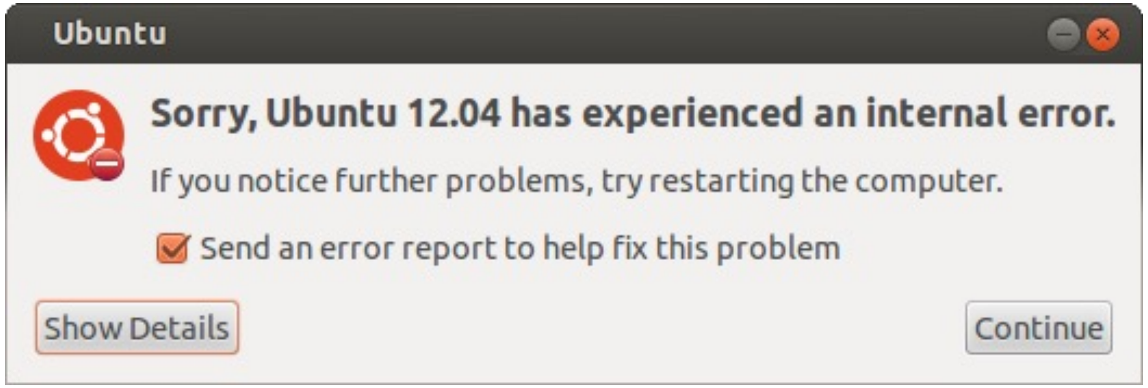
Much is made of the engineering that enables the complex operations of a rover examining the surface of Mars—and rightly so. But even the most advanced robotics are useless if, when the rover rolls out onto the Martian soil, a software glitch causes a communications breakdown and leaves the robot frozen. Whether it is a Mars rover, a deep space probe, or a space shuttle, space operations require robust, practically fail-proof programming to ensure the safe and effective execution of mission-critical control systems.

Just as rovers are rigorously tested in simulated Martian conditions on Earth before actual mission launch, the software components must also be

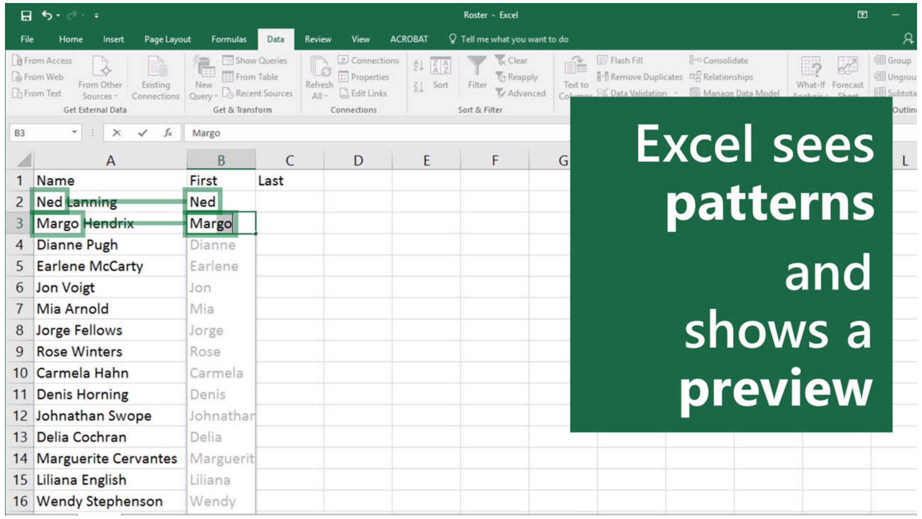
Hard to be perfect, but statistics helps







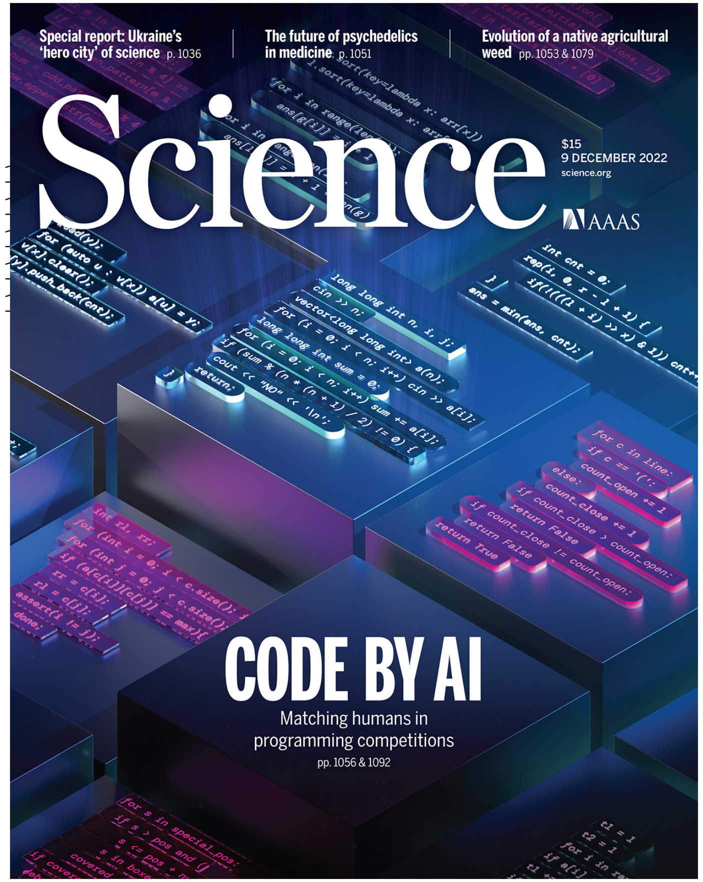
Learn/synthesize small code



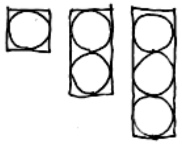
GitHub Copilot

```
# gcc -O3

.L0:
  movq rsi, r9
  movl ecx, ecx
  shrq 32, rsi
  andl 0xffffffff, r9d
  movq rcx, rax
  movl edx, edx
  imulq r9, rax
  imulq rdx, r9
  imulq rsi, rdx
  imulq rsi, rcx
  addq rdx, rax
  jae .L2
  movabsq 0x100000000, rdx
  addq rdx, rcx
.L2:
  movq rax, rsi
  movq rax, rdx
  shrq 32, rsi
  salq 32, rdx
  addq rsi, rcx
  addq r9, rdx
  adcq 0, rcx
  addq r8, rdx
  adcq 0, rcx
  addq rdi, rdx
  adcq 0, rcx
  movq rcx, r8
  movq rdx, rdi
```

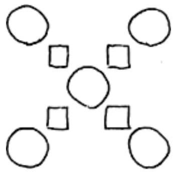
```
# STOKE

.L0:
  shlq 32, rcx
```



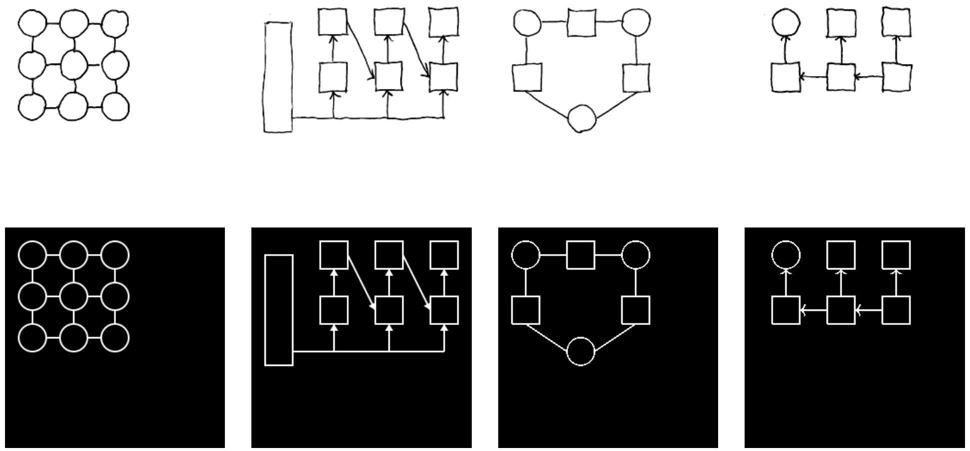
Hand-Drawn Images → Code → Images

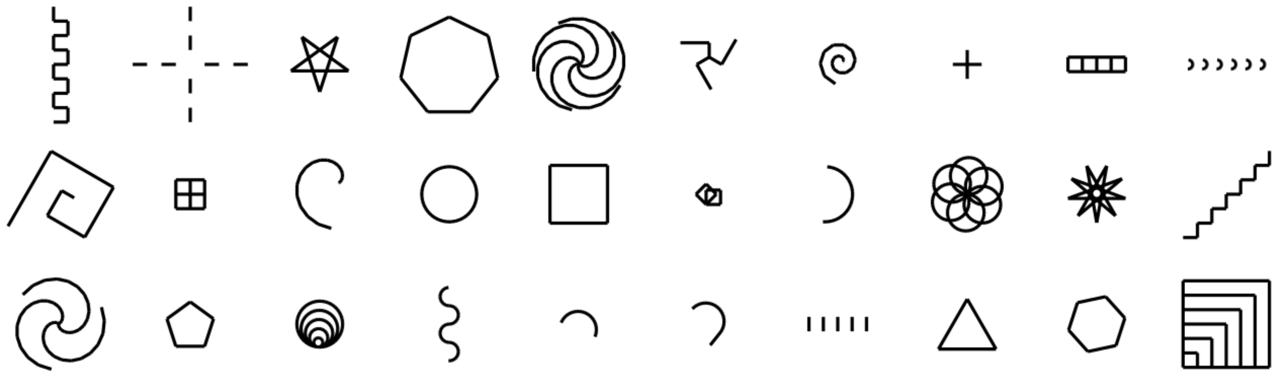


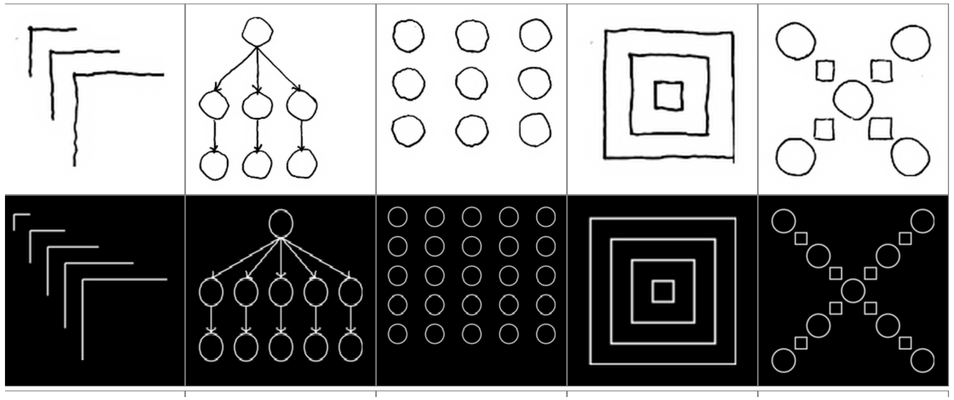
```
for (i < 3)
 rectangle(3*i,-2*i+4,
           3*i+2,6)
 for (j < i + 1)
  circle(3*i+1,-2*j+5)
```



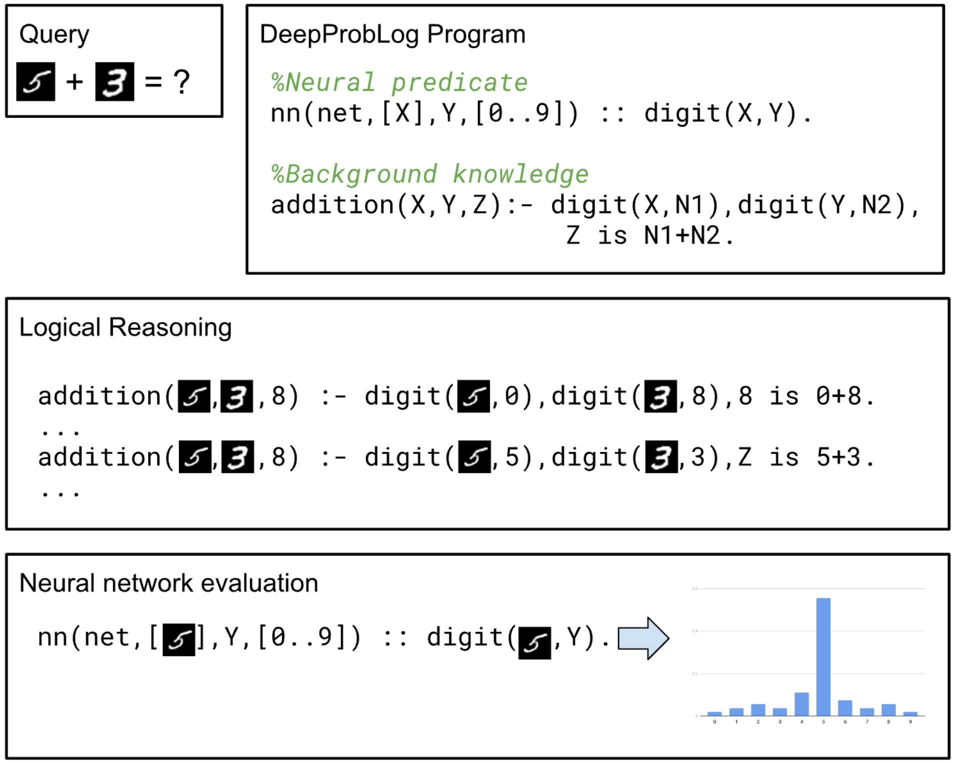
```
reflect(y=8)
 for(i<3)
  if(i>0)
   rectangle(3*i-1,2,3*i,3)
  circle(3*i+1,3*i+1)
```

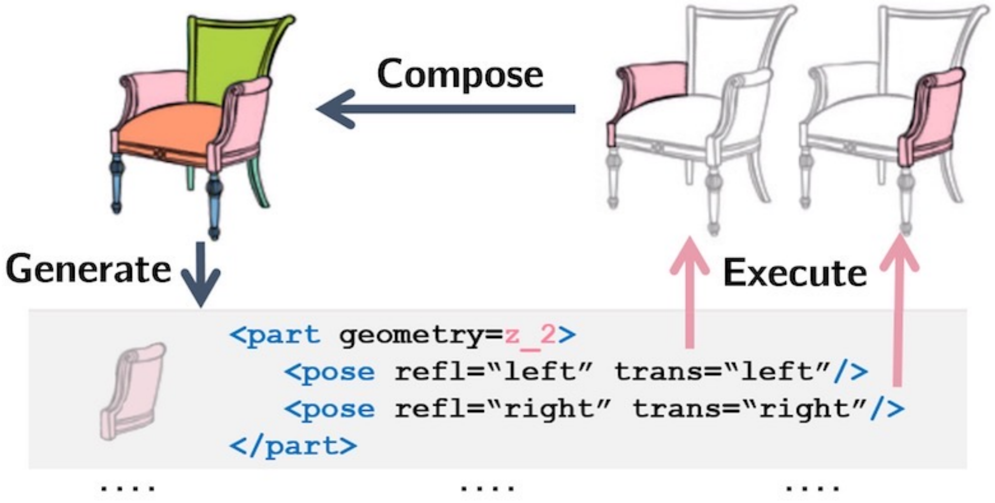


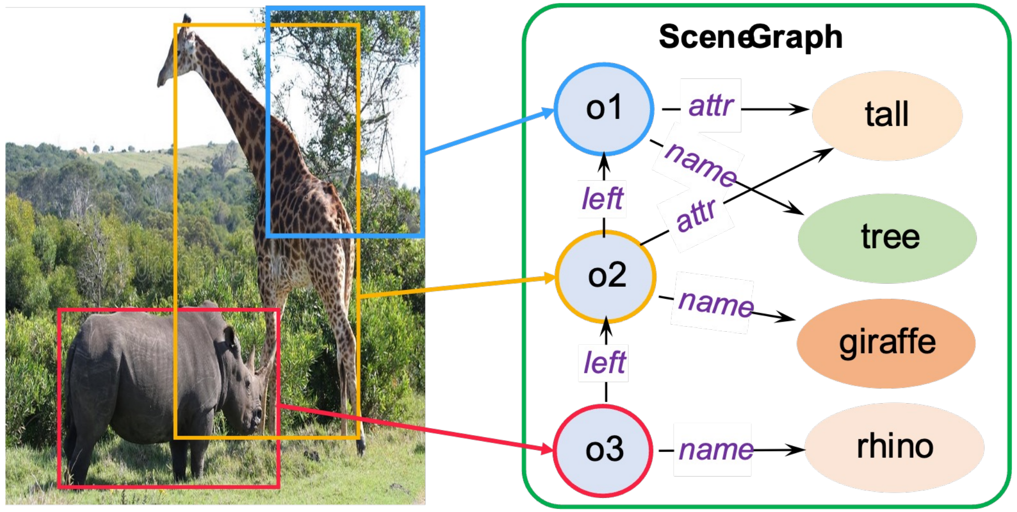




Neuro-Symbolic Systems

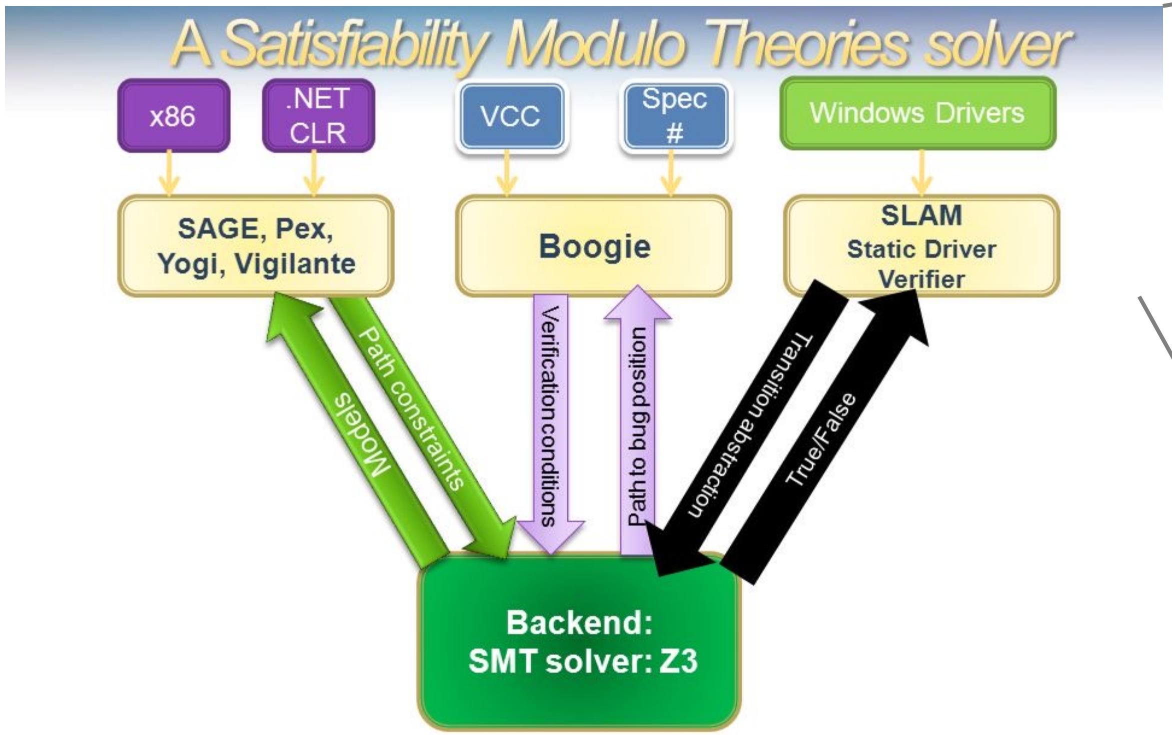


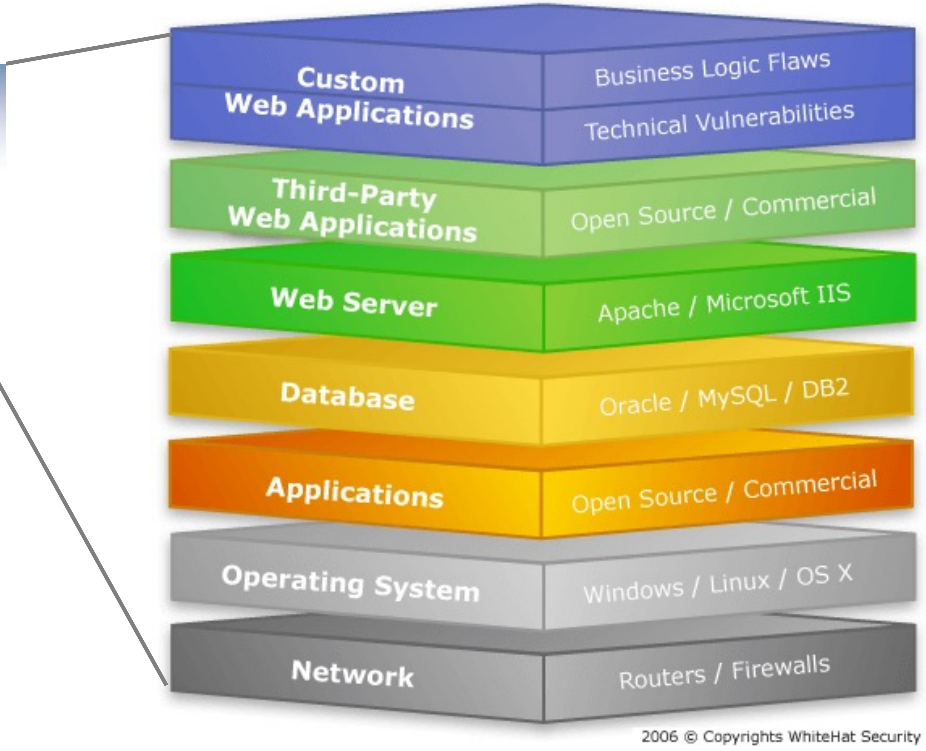




Let’s zoom into the very bottom

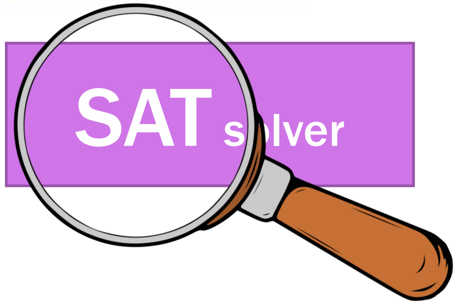
Next next week





Next week

Today



SAT Preliminaries

- **Variables**
  - $w, x, y, z, a, b, c, x_1, x_2, \dots$
- **Literals**
  - Variables or their negations, e.g., $x, \overline{y}$ $(or\ \neg y)$
- **Clauses**
  - Disjunction of literals, e.g., $a \vee x_1 \vee y$
- **Formula**
  - Conjunction of clauses, e.g., $(x_1 \vee \neg y) \wedge (x_2 \vee \neg x_1)$
- **Model**
  - A partial/total mapping from variables to True ($\top$) or False ($\bot$),
  - e.g., $\{x_1 \to \top, x_2 \to \top, y \to \bot\}$
- **Formula can be satisfiable (SAT) or unsatisfiable (UNSAT)**

Notation simplification

- **Literal**
  - Use i to denote x_i
  - Use $-i$ (or $\bar{i}$) to denote $\neg\, x_i$ $(or\ \overline{x_i}\ )$
- **Clause**
  - Use a set $\{x_1, \neg x_2, x_3\}$ to represent a disjunction $x_1 \vee \neg x_2 \vee x_3$
  - Which can be further simplified as $\{1, -2, 3\}$
- **Formula**
  - Use a set $\{c_1, c_2, c_3\}$ to represent a conjunction $c_1 \wedge c_2 \wedge c_3$
  - E.g., $(x_1 \vee \neg x_3) \wedge (x_2 \vee \neg x_1)$ can be simplified as $\{\{1, -3\}, \{2, -1\}\}$
- **Model**
  - Use a set to represent a mapping
  - $\{x_1 \to \top, x_2 \to \bot, x_3 \to \top\}$ can simplified as $\{1, -2, 3\}$

```
c This is a comment
c DIMACS format
p cnf 3 2
1 2 -3 0
-2 3 0
c here is a solution
s 1 -2 3
```

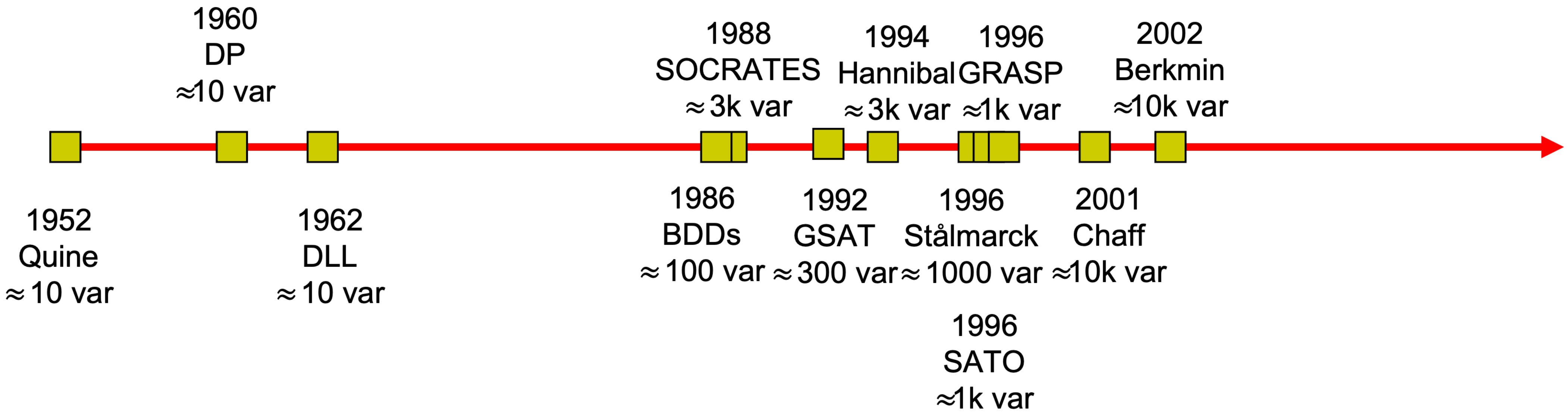
Formula: $(x_1 \vee x_2 \vee \neg x_3) \wedge (\neg x_2 \vee x_3)$

Solution: $\{x_1 \to \top, x_2 \to \bot, x_3 \to \top\}$

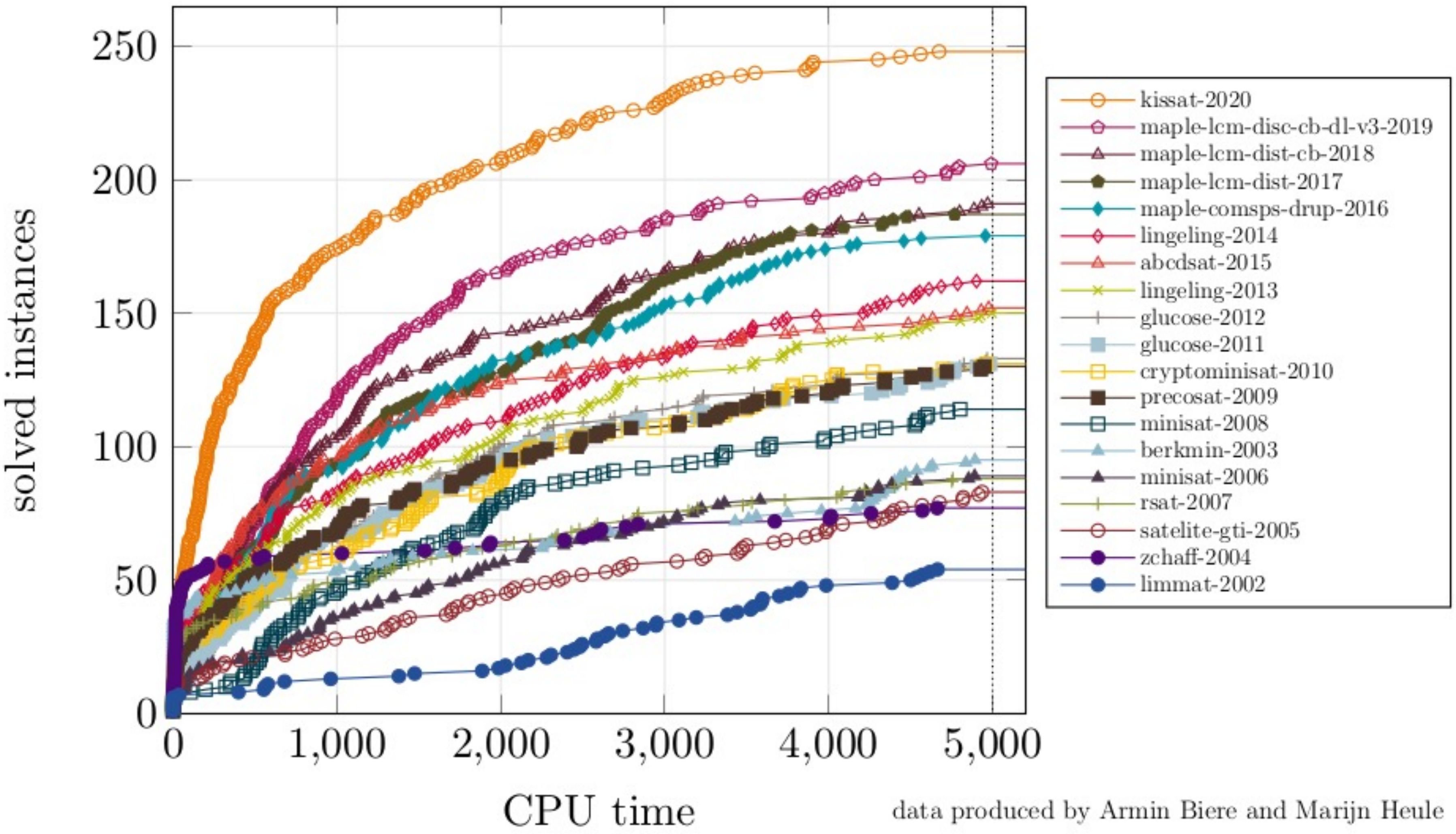
Basic preprocessing

- **Pure literal**
  - A variable x occurs only positively (or only negatively)
  - Remove all clauses containing x
- **Tautology clause**
  - A clause is always true (thus can be removed)
  - E.g., $x_1 \vee x_2 \vee \neg x_1 \vee \cdots$
- **Subsumption**
  - c_1 subsumes c_2 if and only if $c_1 \Rightarrow c_2$ (or $c_1 \subseteq c_2$)
  - E.g., $(x_1 \vee \neg x_3) \Rightarrow (x_1 \vee x_2 \vee \neg x_3)$ (or $\{1, -3\} \subseteq \{1, 2, -3\}$
  - c_2 can be removed safely
- **Unit propagation**
  - A clause contains a single literal l
  - l has to be true if there exists a solution or model

Scalability of (practical) SAT Solving



SAT Competition Winners on the SC2020 Benchmark Suite



Let’s brainstorm a bit …

- **It is easy to check whether an assignment is satisfiable or not**
- **Algorithm-0**
  - Randomly generate an assignment and check if it is a satisfiable solution
- **Algorithm-1**
  - Let’s enumerate all possible assignments, say in lexicographic order
  - E.g., starting with all variables are True, then only one variable is False… then two …
- **Algorithm-2**
  - Once a variable’s truth value has been decided, we can *simplify* the formula
  - We may enumerate in *different* orders

Unit Propagation

- **A.k.a, Boolean Constraint Propagation (BCP)**
  - If a clause consists of a single literal (called unit clause), that literal has to be True.
  - Simplify the formulation, and perform BCP recursively if there is new unit clause(s)

$$\boxed{x_1 \wedge} \; (\neg x_2 \vee \neg x_1) \wedge (x_3 \vee x_2) \wedge (x_1 \vee x_3) \wedge$$

$$\xrightarrow{x_1 = \top}$$

$$\cancel{x_1 \wedge} \; (\neg x_2 \vee \cancel{\neg x_1}) \wedge (x_3 \vee x_2) \wedge \cancel{(x_1 \vee x_3) \wedge}$$

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

$$\xrightarrow{x_2 = \bot}$$

$$\cancel{(\neg x_2) \wedge} \; (x_3 \vee \cancel{x_2}) \wedge$$

$$\xrightarrow{x_3 = \top}$$

$$\cancel{(x_3) \wedge}$$

Empty Formula vs Empty Clause

- **Empty formula is trivially satisfied.**
- **Empty clause cannot be satisfied.**

$$\boxed{(x_1) \land} \quad (\neg x_1) \land \quad \xrightarrow{x_1 = \top} \quad \cancel{(x_1) \land} \quad (\neg \cancel{x_1}) \land$$

Empty formula $\equiv$ no more constraints

Empty clause $\equiv$ no more literals that can be assigned to True

Other basic pre-processings

- **Pure literal**
  - A variable x occurs only positively (or only negatively)
  - Remove all clauses containing x
- **Tautology clause**
  - A clause is always true (thus can be removed)
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- **Subsumption**
  - c_1 subsumes c_2 if and only if $c_1 \Rightarrow c_2$ (or $c_1 \subseteq c_2$)
  - E.g., $(x_1 \vee \neg x_3) \Rightarrow (x_1 \vee x_2 \vee \neg x_3)$ (or $\{1, -3\} \subseteq \{1, 2, -3\}$)
  - c_2 can be removed safely

DPLL Algorithm

Davis–Putnam–Logemann–Loveland (1962)

Algorithm $\texttt{DPLL}(F)$:

- $\boxed{G \leftarrow \texttt{BCP}(F)}$
- **if** $G = \top$ **then return** true
- **if** $G = \bot$ **then return** false
- $\boxed{p \leftarrow \texttt{Choose}(G)}$
- **return** $\underbrace{\texttt{DPLL}(G\{p \mapsto \top\}) \parallel \texttt{DPLL}(G\{p \mapsto \bot\})}_{\text{Better backtracking}}$

Better data structures

Better branching heuristics

Optimizing BCP

- **BCP takes 80-90% of solver time**
- **Classic implementation**
  - For each clause, have counters for satisfied, falsified, and unresolved literals
  - When a literal is set or unset, update counters for all relevant clauses
- **“2 watched literals” trick**
  - A clause does not affect the search if it has two or more non-falsified literals
  - Only need to pick two literals to watch for each clause
- **When either is falsified**
  - Check if there is another non-falsified literal, use that one as the new watched literal
  - Otherwise, the current clause becomes unit clause

Advantages of ”2 watched literals”

- **Fewer clauses are visited when a literal is set**
- **unset is $O(1)$**
  - No literals are falsified
  - Watched literals are unchanged
- **When a literal is frequently “set-then-unset”**
  - Fewer clauses will be affected
  - When a clause is affected for the very first time, another watched literal is chosen

Two popular branching heuristics

Function `ChooseDLIS(`F`)`:
    for *clause* $cl \in F$ **do**
        for *literal* $lit \in cl$ **do**
            count[lit] $\leftarrow$ count[lit] + 1
        end
    end
    return literal w. the max. count

Dynamic Literal Individual Sum (DLIS)

Function `ChooseVSIDS(`F`)`:
    `// initialize scores`
    score[v $\in$ vars] $\leftarrow 0$
    `// when adding a learnt clause`
    for $v \in$ *learnt clause* **do**
        score[v] $\leftarrow$ score[v] + 1
    end
    `// after every N steps`
    for $v \in$ *vars* **do**
        score[v] $\leftarrow \frac{\text{score}[v]}{c}$
    end
    return variable w. the highest score

Variable State Independent Decaying Sum (VSIDS)

Decision Levels

$$\mathcal{F} = (r) \land (\bar{r} \lor s) \land$$
$$(\bar{w} \lor a) \land (\bar{x} \lor \bar{a} \lor b)$$
$$(\bar{y} \lor \bar{z} \lor c) \land (\bar{b} \lor \bar{c} \lor d)$$

- Decisions / Variable Branchings:

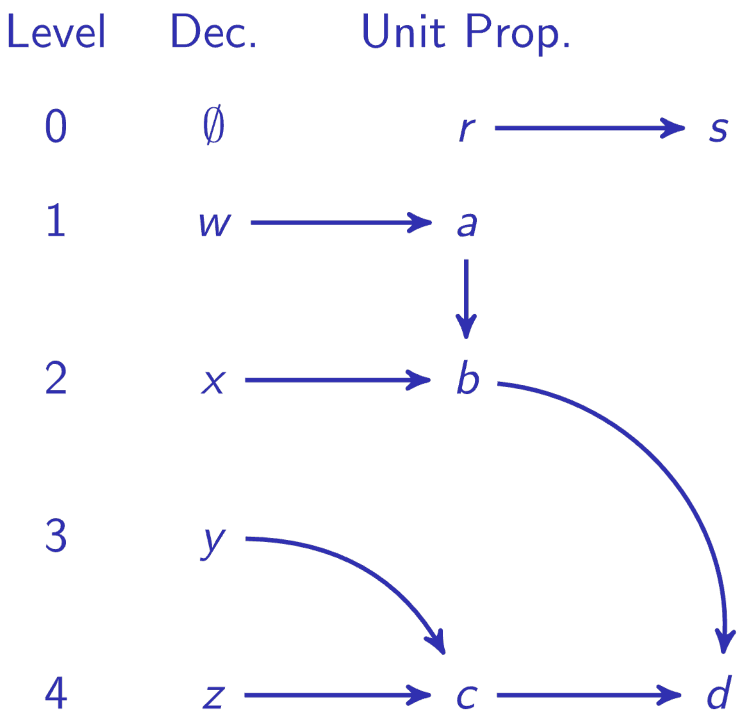
  $w = 1, x = 1, y = 1, z = 1$

$r@0 = 1$

$w@1 = 1$

$x@2 = 1$

$d@4 = 1$



$$\neg b_1 \lor \neg b_2 \lor \cdots \lor \neg b_n \lor h \qquad b_1 \land b_2 \land \cdots \land b_n \Rightarrow h$$

Horn clause: a clause with at most one positive literal

Conflict-driven Clause Learning

Marques-Silva & Sakallah, 1996

$F = \{ c_1, c_2, c_3, c_4, c_5, c_6, \ldots, c_9 \}$

$c_1 : \neg x_1 \lor x_2 \lor \neg x_4$

$c_2 : \neg x_1 \lor \neg x_2 \lor x_3$

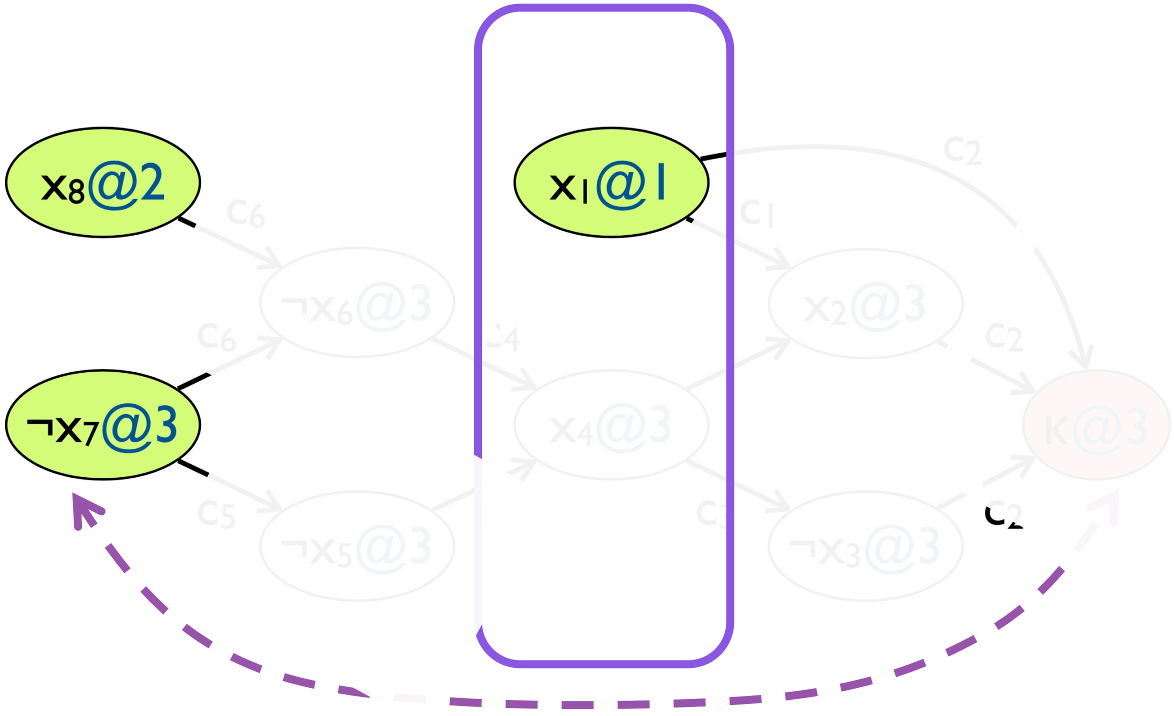
$c_3 : \neg x_3 \lor \neg x_4$

$c_4 : x_4 \lor x_5 \lor x_6$

$c_5 : \neg x_5 \lor x_7$

$c_6 : \neg x_6 \lor x_7 \lor \neg x_8$

$x_1 = \top, x_4 = \top$

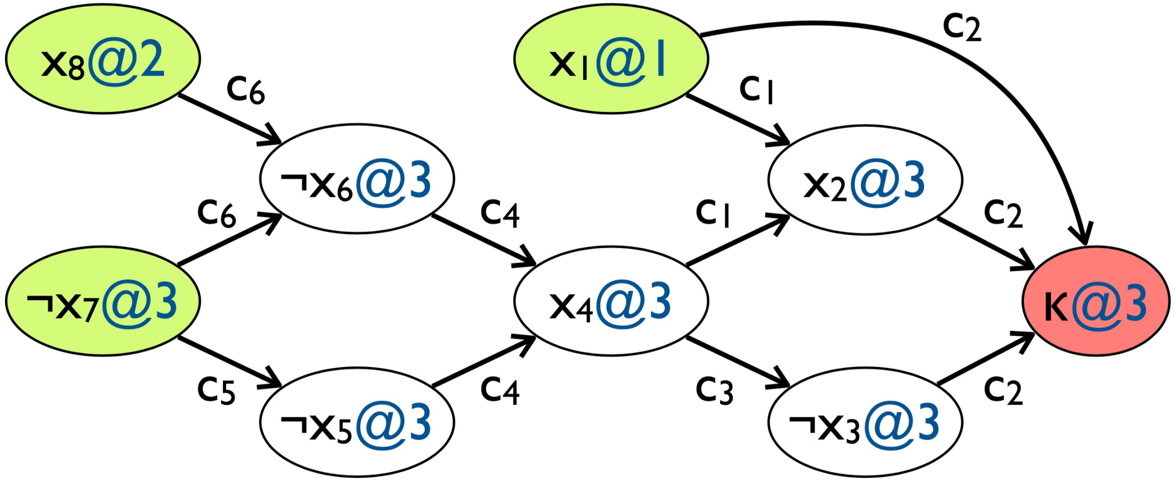


$\neg x_1 \lor \neg x_4 \longleftarrow NOT\ (x_1 = \top \land x_4 = \top)$

$\neg x_1 \lor \neg x_8 \lor x_7 \longleftarrow NOT\ (x_1 = \top \land x_8 = \top \land x_7 = \bot)$

Many steps later...

Non-chronological backtracking



$x_1@1 = \top$

$x_8@2 = \top$

$x_7@3 = \bot$

(failed)

$\neg x_1 \vee \neg x_8 \vee x_7$

$x_1@1 = \top$

$x_8@2 = \top$

$x_7@2 = \top$

$\neg x_1 \vee \neg x_4$

$x_1@1 = \top$

$x_4@1 = \bot$

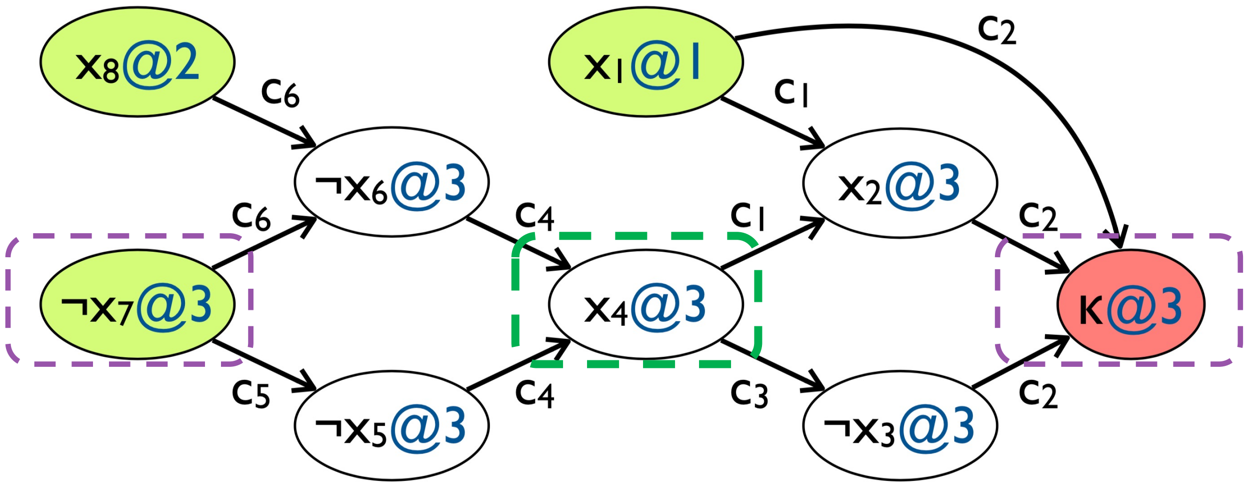
$$C_{learnt} = l_{d_1} \vee l_{d_2} \vee \cdots \vee l_{d_k}$$

$$where\ d_1 < d_2 < \cdots < d_k$$

Backtrack to level d_{k-1} so that C will become a unit clause immediately

How to choose a proper conflict?

- **Unique Implication Point (UIP)**
  - A single node at level d such that all paths from the current decision literal $(lit@d)$ to the conflict $(k@d)$
  - Obviously, the source node (lit) and the sink node (k) are UIPs.
- **First UIP strategy**
  - Pick the conflict that consists of the closest UIP to the conflict node

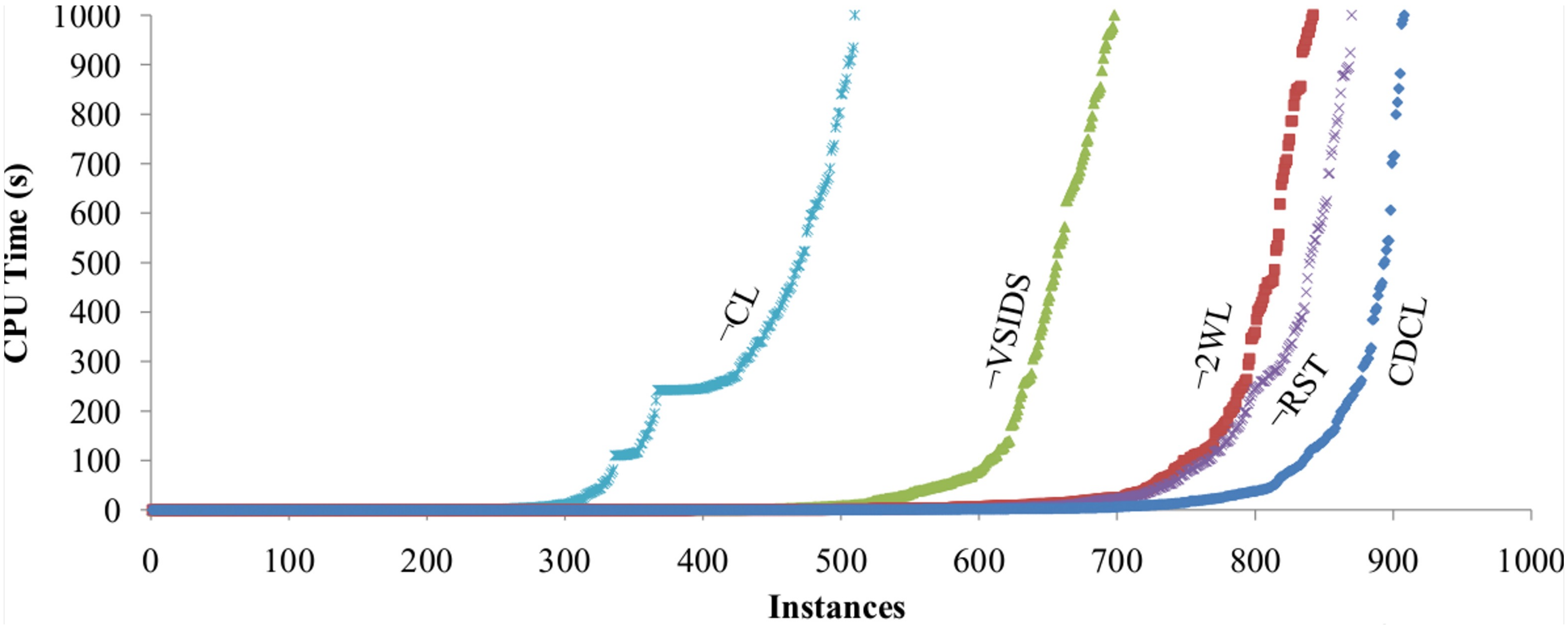


Restart

- **Restart from scratch once in a while**
- **Why useful at all?**
  - (Some) Learnt clauses will be kept
  - Even with same heuristics, the search will go to a different direction
  - With learnt clauses, extra pre-processing (or “in-processing”) can be performed

Ablation Study of Modern CDCL Solver

Importance of major features: Clause Learning > VSIDS > 2WL > Restart



[Source: Katebi, Skallah & Marques-Silva 2011]

Well-known SAT solvers

- Chaff (2002)
  - https://www.princeton.edu/~chaff/zchaff.html
- MiniSat (2005)
  - http://minisat.se/
- Glucose (2009)
  - https://www.labri.fr/perso/lsimon/glucose/
- CaDiCaL (2017)
  - http://fmv.jku.at/cadical/
- Kissat (2020)
  - https://github.com/arminbiere/kissat

Proof

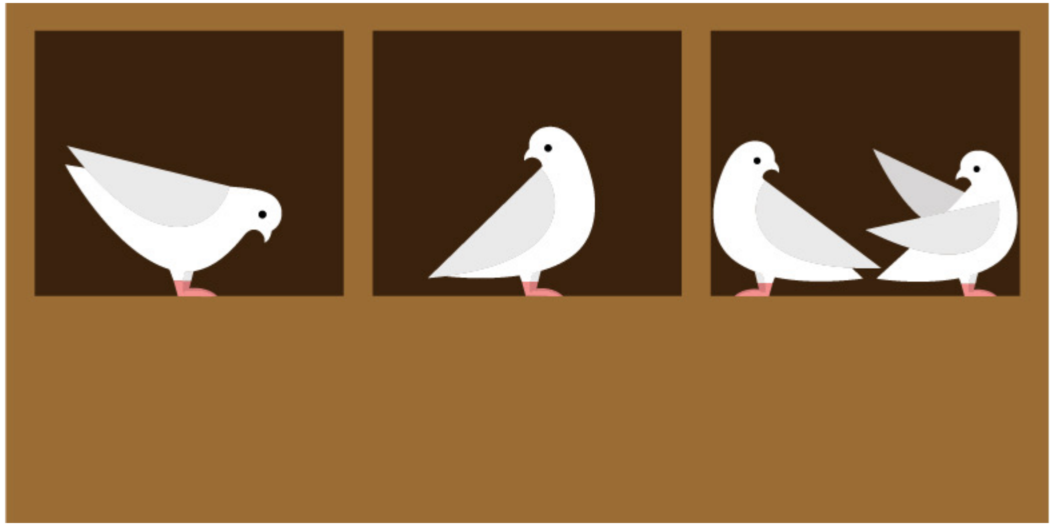
- **A satisfiable solution is easy to check/verify**
- **What if a solver claims UNSAT?**
  - A sequence of resolution ends up with an empty clause
  - CDCL is essentially constructing a resolution-based proof when an instance is UNSAT
  - The proof size could be quite large
  - For the pigeonhole problem, the resolution-based proof size is exponential

Armin Haken, *The intractability of resolution*, Theoretical Computer Science, 1985
https://www.sciencedirect.com/science/article/pii/0304397585901446

Haken's lower bound (slides): https://www.ti.inf.ethz.ch/ew/courses/extremal04/raemy.pdf

Limitation of CDCL

Pigeonhole principle



If we put $n+1$ pigeons into n holes, there exists at least one hole with more than one pigeons.

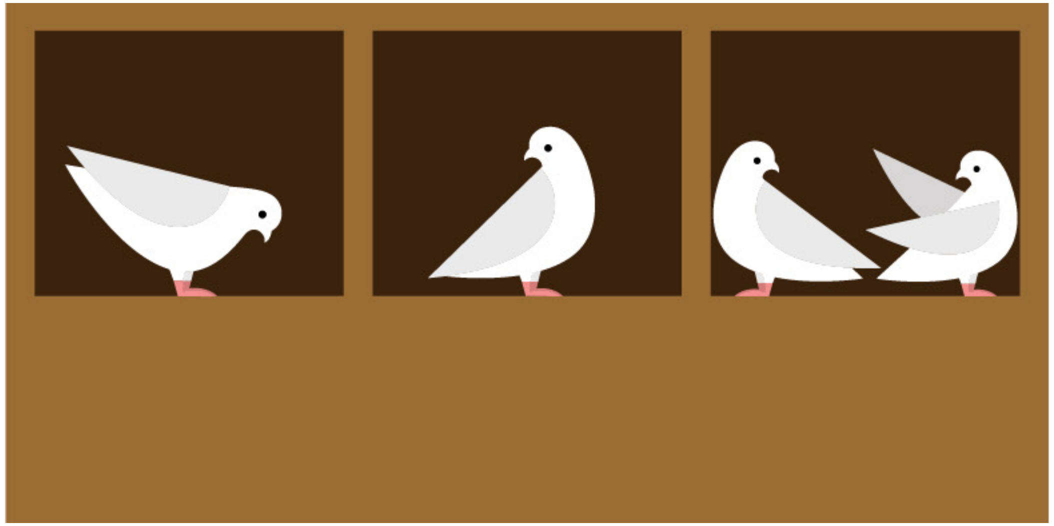
How to encode PHP as a SAT solving problem?

CDCL-based SAT solvers suffer from solving PHP instances

Satisfiability vs Validity

- **Satisfiability**
  - There exists some assignment so that the formula is true.
  - $\exists x_1, x_2, \dots, x_n.\, \phi(x_1, \dots, x_n)$
- **Validity**
  - For all assignments, the formula is true.
  - $\forall x_1, x_2, \dots, x_n.\, \phi(x_1, \dots, x_n)$
- **The negation of one is equivalent to the other**
  - $NOT\ \left(\exists x_1, x_2, \dots, x_n.\, \phi(x_1, \dots, x_n)\right) \equiv \forall x_1, x_2, \dots, x_n.\, \neg\ (\phi(x_1, \dots, x_n))$
  - $NOT\ \left(\forall x_1, x_2, \dots, x_n.\, \phi(x_1, \dots, x_n)\right) \equiv \exists x_1, x_2, \dots, x_n.\, \neg\ (\phi(x_1, \dots, x_n))$

Pigeonhole Principle



"For all possible arrangements, some hole contains one or more pigeons."

Tautology

Negation

"There exists an arrangement, no hole contains more than one pigeons."

UNSAT

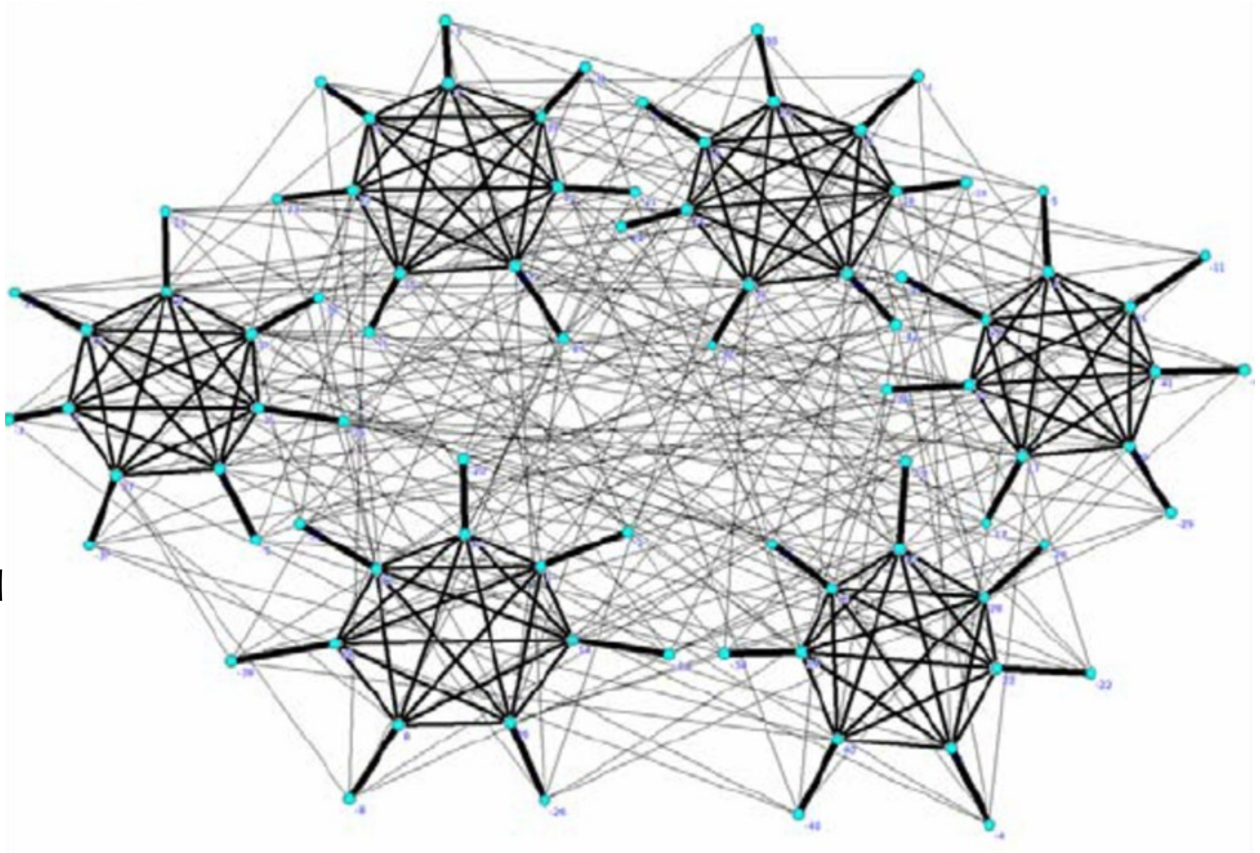
Rephrase

UNSAT

"There exist an arrangement, each hole contains one (or less) pigeon."

SAT Encoding of Pigeonhole problem

- **N+1 pigeons, N holes**
- **Boolean variable $x_{i,j}$**
  - the i-th pigeon is placed in the j-th hole
- **Each pigeon should be in some hole**
  - $x_{i,1} \vee x_{i,2} \vee \cdots \vee x_{i,n}$
  - N+1 clauses
- **No hole contains more than one pigeon**
  - Any pair of pigeons should not be in the same hol
  - $\neg x_{i,j} \vee \neg x_{k,j}$ where $i \neq k$
  - For each hole, $\frac{(n+1)*n}{2}$ clauses



Demo: try Minisat on Pigeonhole

- Minisat solver
  - http://minisat.se/
- PHP constraints generation
  - https://user.it.uu.se/~tjawe125/software/pigeonhole/