

Lecture 24: Satisfiability Modulo Theories and Cook–Levin

*Harvard SEAS - Fall 2024**2024-11-26*

1 Announcements

Recommended Reading:

- De Moura & Bjørner:
<https://cacm.acm.org/magazines/2011/9/122785-satisfiability-modulo-theories/abstract>

Announcements:

- PS9 due Wed 12/4
- No section this week
- Final exam Thu 12/19, 9am. Cheat sheet allowed; details TBA.
- Practice exams to be released and review sessions and OH to be announced 12/4.
- Late revision videos will be accepted at half credit.
- CS1200 merch ideas due Sun 12/1.
- Today's material is mostly for fun/culture; you do not need to be able to work with it at a technical level, but it may help reinforce some of the earlier material in the course.
- Q evaluations open; please fill out.
- PS7 feedback: median 9hrs, 75th percentile 10hrs. Resolution problem a bit tedious, 3d complete matching input format ambiguous.
- SRE6 feedback: 89% of senders and 93% of receivers found it useful. Visualizations very helpful; DCE students could use ability to share screen.
- Happy Thanksgiving!

2 Program Verification and Analysis

A dream (especially for TFs in CS courses!) is that we could just write a mathematical specification of what a program P should do, such as the following, and then automatically verify that a program meets the specification:

$$\text{Spec} : \forall A, \ell, u, K \ (0 \leq \ell \leq u, \forall i \ A[i-1] \leq A[i]) \rightarrow (P(A, \ell, u, K) = \text{yes} \leftrightarrow \exists i \in [\ell, u] \ A[i] = K) .$$

More precisely, our dream is an algorithm V that given a specification Spec and a program P , $V(\text{Spec}, P)$ will always tell us whether or not P satisfies Spec .

Q: Why is the dream not achievable?

A:

Like with the NP-complete problems, this does not mean we completely give up on building useful software tools to analyze and verify programs. But it does mean that all such tools must have one or more of the following limitations:

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Nevertheless, the tools for program verification have grown in power and sophistication over the years, and today we will study one of the most powerful approaches, known as Satisfiability Modulo Theories.

3 Constraint Satisfaction Modulo Theories

Constraint satisfaction problems (CSPs) are a general framework for defining computational problems, where the instances are a set of constraints over a finite set of variables z_0, \dots, z_{n-1} and we ask to find an assignment to the variables that satisfies all of the constraints, or declare that the set of constraints is unsatisfiable. SAT is an example, where the constraints allowed are *disjunctions* of literals and we ask whether there is a *Boolean* assignment to the variables that satisfies all of the constraints. Here we consider a much more general formulation where (a) the variables can take values in an arbitrary domain \mathcal{D} and (b) the constraints can come from an arbitrary collection \mathcal{P} .

Definition 3.1. A *theory* \mathcal{T} consists of a domain \mathcal{D} and a collection \mathcal{P} of predicates $p : \mathcal{D}^k \rightarrow \{0, 1\}$, $k \geq 0$.

Let's see an example.

The Theory of Naturals. $\mathcal{D} = \mathbb{N}$, with the following predicates and their negations.

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An example instance of a CSP Modulo the Theory of Naturals is the following:

$$\begin{aligned} x \neq 0, \quad x_2 = x \times x, \quad x_4 = x_2 \times x_2, \\ y \neq 0, \quad y_2 = y \times y, \quad y_4 = y_2 \times y_2, \\ z \neq 0, \quad z_2 = z \times z, \quad z_4 = z_2 \times z_2, \\ x_4 + y_4 = z_4 \end{aligned}$$

Q: What Diophantine Equation does the above look for solutions to?

A: Let's turn to some solvable examples:

The Theory of Disjunctions. $\mathcal{D} = \{0, 1\}$, with the predicate family $\mathcal{P} = \{p_{k,\ell} : k, \ell \in \mathbb{N}\}$, where

$$p_{k,\ell}(x_0, \dots, x_{k+\ell-1}) = [x_0 \vee \dots \vee x_{k-1} \vee \neg x_k \vee \dots \vee \neg x_{k+\ell-1}].$$

CSPs Modulo The Theory of Disjunctions is just another way of describing SAT.

The Theory of Bitvectors of length w . Here the domain is $\mathcal{D}_w = \{0, 1, \dots, 2^w - 1\} \equiv \{0, 1\}^w$, with the following predicates and their negations

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Q: Why is this theory solvable?

A:

As we see in this example, sometimes the domain and/or the predicates in the Theory have one or more size parameters, like the word size w , which may affect the complexity of solving the problem.

The Theory of Difference Arithmetic: $\mathcal{D} = \mathbb{Q}$, with predicates

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Here, even though the domain \mathcal{D} is infinite, it is a solvable theory and in fact can be solved (via single-source shortest paths in digraphs that can have both positive and negative edge weights).

The general definition of CSPs Modulo a Theory $\mathcal{T} = (\mathcal{D}, \mathcal{P})$ is as follows:

Input	: A sequence $z = (z_0, \dots, z_{n-1})$ of n <i>theory variables</i> , and a sequence of <i>theory predicates</i> $P_0(z), \dots, P_{m-1}(z)$, each of which is obtained by applying a predicate $p \in \mathcal{P}$ to a sequence $(z_{i_0}, \dots, z_{i_{k-1}})$ of theory variables.
Output	: An assignment

Computational Problem ConstraintSatisfactionInT

4 Satisfiability Modulo Theories

In *Satisfiability Modulo Theories*, we combine SAT over Boolean variables with predicates from a theory, allowing us to have a system of constraints like the following over the Theory of Difference Arithmetic, where x_0, \dots, x_n are propositional (i.e. Boolean) variables, s_0, \dots, s_n are rational variables, and $v_0, \dots, v_{n-1}, t \in \mathbb{Q}$ are constants given in the input:

- $s_0 = 0$,
- $x_i \rightarrow s_{i+1} = s_i + v_i$ for $i = 0, \dots, n-1$,
- $\neg x_i \rightarrow s_{i+1} = s_i$ for $i = 0, \dots, n-1$,
- $s_n = t$

Q: What familiar problem do the above constraints encode?

A:

In general, an SMT instance is given by CNF formula where some of the variables are replaced by predicates over theory variables. Formally:

Input	: A CNF formula $\varphi(x_0, \dots, x_{n_p-1}, y_0, \dots, y_{n_q-1})$ on n_p <i>propositional variables</i> and n_q <i>auxiliary variables</i> , a sequence $z = (z_0, \dots, z_{n_t-1})$ of n_t <i>theory variables</i> , and a sequence of n_q <i>theory predicates</i> $P_0(z), \dots, P_{n_q-1}(z)$, each of which is obtained by applying a predicate $p \in \mathcal{P}$ to a sequence $(z_{i_0}, \dots, z_{i_{k-1}})$ of theory variables.
Output	: Assignments $\alpha \in \{0, 1\}^{n_p}$, $\beta \in \mathcal{D}^{n_t}$ such that

$$\varphi(\alpha, P_0(\beta), \dots, P_{n_q-1}(\beta)) = 1,$$

if such assignments exist.

Computational Problem SatisfiabilityModuloT

Figure 1: Evaluating a solution (α, β) to an SMT instance $(\varphi, P_0, \dots, P_{n_q-1})$

Example: As an example, let's write a Subset Sum instance with $n = 3$, $(v_0, v_1, v_2) = (1, 3, 9)$ and $t = 10$ using this formalism:

Theorem 4.1. *For every theory \mathcal{T} , Satisfiability Modulo $\mathcal{T} = (\mathcal{D}, \mathcal{P})$ is solvable iff Constraint Satisfaction Modulo $\mathcal{T}' = (\mathcal{D}, \mathcal{P} \cup \neg\mathcal{P})$ is solvable, where $\neg\mathcal{P}$ includes the negations of all predicates in \mathcal{P} .*

Proof sketch.

\Rightarrow

\Leftarrow We give a (exponential-time) reduction from Satisfiability Modulo \mathcal{T} to Constraint Satisfaction Modulo \mathcal{T}' :

□

Like SAT Solvers, there has been an enormous amount of engineering effort put into designing highly optimized SMT Solvers, which perform well on many useful real-world instances, even when the theory \mathcal{T} is unsolvable. You can play around with one such solver, Z3, at <https://microsoft.github.io/z3guide/>.

5 Using SMT Solvers for Program Analysis

Let's see an example of how SMT Solvers (for “Satisfiability Modulo Theories”), are used for finding bugs in programs. Consider the following program for Binary Search:

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1 BinarySearch( $A, \ell, u, k$ )
  Input      : Integers  $0 \leq \ell \leq u$ , a sorted array  $A$  of length at least  $u$ , a key  $k$ 
  Output     : yes if  $k \in \{A[\ell], A[\ell + 1], \dots, A[u - 1]\}$ , no otherwise
2 while  $\ell < u$  do
3    $m = (\ell + u)/2$ ;
4   if  $A[m] = k$  then
5     return yes
6   else if  $A[m] > k$  then
7      $\ell = \ell$ ;  $u = m$ 
8   else  $\ell = m + 1$ ;  $u = u$ ;
9   assert  $0 \leq \ell \leq u$ ;
10 return no

```

This looks like a correct implementation of binary search, but to be sure we have added an assert command in Line 9 to make sure that we got all of our arithmetic right and maintain the invariant that $0 \leq \ell \leq u$.

For our `BinarySearch()` program here, we will consider whether there are inputs that make the assertion fail *within the first two iterations of the loop*. To do this, we will have the following variables in our SMT formula:

- x_i for $i = 2, \dots, 10$: propositional variable representing whether or not we execute line i in the first iteration of the loop.
- x'_i for $i = 2, \dots, 10$: propositional variable representing whether or not we execute line i in the second iteration of the loop.
- x_f : propositional variable representing whether the assertion fails during the first two iterations of the loop. (So x_f will be false if the program either halts with an output during the first two iterations or reaches the end of the second iteration without the assertion failing.)
- ℓ, u, k : integer variables representing the input values for ℓ, u, k
- ℓ', u' : integer variables representing the values of ℓ, u if and when Line 9 is reached in the first iteration of the loop.
- ℓ'', u'' : integer variables representing the values of ℓ, u if and when Line 9 is reached in the second iteration of the loop.
- m, m' : integer variables representing the values assigned to m in the first and second iterations of the loop.
- a, a' : representing values of $A[m]$ and $A[m']$.

We then construct our formula as the conjunction of the following constraints, corresponding to the input preconditions (Constraint 1–2), the control flow and assignments made by the program (Constraints 3–31), and asking for the assertion to fail (Constraint 32).

1. $(0 \leq \ell) \wedge (\ell \leq u)$
2. $((m \leq m') \rightarrow (a \leq a')) \wedge ((m \geq m') \rightarrow (a \geq a'))$
3. (x_2)
4. $(x_2 \wedge (\ell < u)) \leftrightarrow x_3$
5. $(x_2 \wedge \neg(\ell < u)) \leftrightarrow x_{10}$
6. $x_3 \rightarrow ((m = (\ell + u)/2) \wedge x_4)$
7. $(x_4 \wedge (a = k)) \leftrightarrow x_5$
8. $(x_4 \wedge \neg(a = k)) \leftrightarrow x_6$
9. $x_5 \rightarrow \neg x_f$
10. $(x_6 \wedge (a > k)) \leftrightarrow x_7$
11. $(x_6 \wedge \neg(a > k)) \leftrightarrow x_8$
12. $x_7 \rightarrow ((u' = m) \wedge (\ell' = \ell) \wedge x_9)$
13. $x_8 \rightarrow ((\ell' = m + 1) \wedge (u' = u) \wedge x_9)$
14. $x_7 \vee x_8 \leftrightarrow x_9$
15. $(x_9 \wedge \neg((0 \leq \ell') \wedge (\ell' \leq u'))) \rightarrow x_f$
16. $(x_9 \wedge (0 \leq \ell') \wedge (\ell' \leq u')) \leftrightarrow x'_2$
17. $x_{10} \rightarrow \neg x_f$
18. $(x'_2 \wedge (\ell' < u')) \leftrightarrow x'_3$
19. $(x'_2 \wedge \neg(\ell' < u')) \leftrightarrow x'_{10}$
20. $x'_3 \rightarrow ((m' = (\ell' + u')/2) \wedge x'_4)$
21. $(x'_4 \wedge (a' = k)) \leftrightarrow x'_5$
22. $(x'_4 \wedge \neg(a' = k)) \leftrightarrow x'_6$
23. $x'_5 \rightarrow \neg x_f$
24. $(x'_6 \wedge (a' > k)) \leftrightarrow x'_7$
25. $(x'_6 \wedge \neg(a' > k)) \leftrightarrow x'_8$
26. $x'_7 \rightarrow ((u'' = m') \wedge (\ell'' = \ell') \wedge x'_9)$
27. $x'_8 \rightarrow ((\ell'' = m' + 1) \wedge (u'' = u') \wedge x'_9)$
28. $x'_7 \vee x'_8 \leftrightarrow x'_9$
29. $(x'_9 \wedge \neg((0 \leq \ell'') \wedge (\ell'' \leq u''))) \rightarrow x_f$
30. $(x'_9 \wedge (0 \leq \ell'') \wedge (\ell'' \leq u''))) \rightarrow \neg x_f$
31. $x'_{10} \rightarrow \neg x_f$
32. x_f

To apply an SMT Solver, however, we need to select a “theory” that tells us the domain that the theory variables range over and how to interpret the operations and (in)equality symbols. If we use The Theory of Natural Numbers, then we will find out that φ is *unsatisfiable*, because Algorithm 10 is a correct instantiation of Binary Search over the natural numbers.

However, if we implement Algorithm 10 in C using the `unsigned int` type, then we should not use the theory of natural numbers, but use the Theory of Bitvectors *with modular arithmetic*, because C `unsigned int`’s are 32-bit words, taking values in the range $\{0, 1, 2, \dots, 2^{32} - 1\}$ with modular arithmetic. And in this case, an SMT Solver will find that the formula is *satisfiable*! One satisfying assignment will have:

1. $\ell = 2^{31}$
2. $u = 2^{31} + 2$
3. $m = (\ell + u)/2 =$
4. $a = 0, k = 1$
5. $\ell' = \ell = 2^{31}$
6. $u' = m + 1 =$

This violates the assertion that $\ell' \leq u'$ — a genuine bug in our implementation of binary search!

6 The Cook–Levin Theorem

Now we’ll see how the ideas used for the Binary Search example above can be generalized to perform automatic program analysis of an *arbitrary* Word-RAM program via Satisfiability Modulo the Theory of Bitvectors. We will then use that to give a proof (sketch) of the Cook–Levin Theorem.

We consider the following very general problem:

Input	: A Word RAM program P , an array of natural numbers $x = (x_0, \dots, x_{n-1})$ and parameters $w, m, t \in \mathbb{N}$.
Output	: An array $y = (y_0, \dots, y_{m-1})$ of natural numbers y such that: <ol style="list-style-type: none"> 1. $P[w]$ halts without crashing on input (x, y) within t steps, and 2. $P[w](x, y) = 1$, if such a y exists.

Computational Problem WordRAMSatisfiability

Many debugging problems can easily be reduced to WordRAMSatisfiability, if we fix bounds on the input length and the running time that we care about. For example, if we take $n = 0$ and modify P to output 1 only when an arithmetic overflow occurs, then WordRAMSatisfiability will tell us whether there is an input y of length m that causes an arithmetic overflow within t steps.

Theorem 6.1. *WordRAMSatisfiability can be reduced to Satisfiability Modulo the Theory of Bitvectors. Given an instance (P, x, w, m, t) of WordRAMSatisfiability, the (mapping) reduction produces an SMT instance with the same word size parameter w and runs in time polynomial in $|P|$, $|x|$, m , and t .*

Proof sketch. Given a WordRAMSatisfiability instance (P, x, w, m, t) , we construct our SMT instance very similarly to the binary search example:

- Propositional variables:
- Theory variables:
- Constraints:

□

Now let's use this to prove the Cook–Levin Theorem.

Theorem 6.2. *For every problem $\Pi \in \text{NP}_{\text{search}}$ $\Pi \leq_p \text{WordRAMSatisfiability}$. Specifically, an instance x of Π of bitlength N maps to an instance of WordRAMSatisfiability with $n = N$, $m = N^{O(1)}$, $t = N^{O(1)}$, and $w = O(\log N)$.*

Proof sketch.

□

Theorem 6.3. *Satisfiability Modulo the Theory of Bitvectors reduces to SAT in time polynomial in the length of the input and 2^w .*

There is a more efficient reduction that has complexity polynomial in w , but we don't need it because Theorem 6.2 gives us word length $w = O(\log N)$.

Proof sketch.

□

Combining Theorems 6.2, 6.1, and 6.3 shows that SAT is $\text{NP}_{\text{search}}$ -hard. Thus, we have completed the proof of:

Theorem 6.4 (Cook–Levin Theorem). *SAT is $\text{NP}_{\text{search}}$ -complete.*