PythonFromScratch

Scalable Static Analysis via Symbolic Execution & Barrier Certificates

Technical Deep Dive

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Goal: Sound bug detection for Python at scale
Approach: Z3-based symbolic execution + 5-layer barrier synthesis
Result: 67 bug types, 31 true positives in DeepSpeed (700 files)

System Architecture: 4-Stage Pipeline

Stage 1: Frontend (Python → IR)

- Bytecode compilation via `compile()`
- CFG construction with basic blocks
- SSA form conversion for def-use chains
- Call graph extraction (intra/interprocedural)

Stage 2: Symbolic Execution Engine

- Z3 SMT solver for path constraints
- Path explosion mitigation: loop bounds (default 3), depth limits (default 50)
- Taint tracking: sources (stdin, network, files) → sinks (eval, SQL, etc.)
- Interprocedural summaries with context sensitivity

Stage 3: Bug Detection (67 Types)

- Security: Injection (9), XSS/CSRF (5), Deserialization (4), Crypto (8), Network (7)
- Logic: Bounds, Div-by-zero, Null ptr, Type errors, Assert violations
- Confidence scoring: Path feasibility $\times$ Constraint satisfiability $\times$ Taint flow

Stage 4: Barrier Certificate Verification

- Synthesize $B(x)$ s.t. $B(x) \geq 0$ on initial, $B(x) < 0$ on unsafe, inductive
- 5-layer architecture: SOS/SDP (L1-2) + CEGAR (L3) + Learning (L4) + IC3 (L5)
- Output: **BUG** (counterexample), **SAFE** (certificate), **UNKNOWN**

Z3 SMT Solver: Symbolic State

Symbolic State

$$\Sigma = \langle \mathsf{pc}, \sigma, \pi, \tau \rangle$$

Components

- pc: path condition (Z3 formula)
- σ: symbolic store (variables)
- π: heap model (objects)
- τ: taint tracking map

Z3 SMT Solver: Example

Code

```
if x > 0:  y = 1 / x
```

Analysis

Path condition: pc $= (x > 0)$

Bug condition: $(x = 0)$

Z3 query: Is $(x > 0) \wedge (x = 0)$ satisfiable?

Result: UNSAT $\Rightarrow$ Safe!

Z3: Solver Strategies

Incremental Solving

- Use `push()`/`pop()` for branches
- Reuse constraint context
- Avoid redundant work

Theory Selection

- Bit-vectors for integers
- Array theory for collections
- Quantifiers for loops

Z3: Performance Management

Timeout Strategy

- Per-query timeout: 5 seconds
- Fallback to under-approximation
- Cache unsatisfiable cores

Concolic Validation

- Extract concrete values from SAT
- Execute with concrete inputs
- Validate bug actually triggers

Interprocedural Analysis

The Challenge

Real programs have thousands of functions.

We need to analyze function interactions!

Call Graph Construction

1. Parse all files $\rightarrow$ AST
2. Extract function definitions
3. Resolve calls (direct & indirect)
4. Build call graph

Context Sensitivity

k-CFA (Call-Flow Analysis)

Track last k call sites:

Levels

- $k = 0$: context-insensitive
- $k = 1$: track caller
- $k = 2$: track caller + caller's caller

Default: $k = 2$

Function Summaries

Summary Format

$$\mathrm{Sum}(f) = \langle \mathrm{Pre}, \mathrm{Post}, \mathrm{Mod}, \mathrm{Taint} \rangle$$

Components

Pre: Input preconditions

Post: Output postconditions

Mod: Modified state

Taint: Propagation rules

Compositional Analysis

Bottom-Up Strategy

1. Analyze leaves first
2. Propagate summaries upward
3. Each function analyzed once!

Result

6,208 functions in 38 seconds

Barrier Certificates: The Problem

Given

Program states X

Initial states $I \subseteq X$

Unsafe states $U \subseteq X$ (bugs)

Transition τ (program semantics)

Prove: I never reaches U

Barrier Certificates: The Solution

Find Function $B : X \to \mathbb{R}$

Initial: $B(x) \geq 0$ for all $x \in I$

Unsafe: $B(x) < 0$ for all $x \in U$

Inductive: If $B(x) \geq 0$ and $x \to x'$,
then $B(x') \geq 0$

$\Rightarrow$ **SAFE!**

Polynomial Barriers: Template

Polynomial Form

$$B(x) = \sum_i c_i \cdot m_i(x)$$

Components

$m_i(x)$ = monomials

e.g., $1, x, y, x^2, xy, y^2$

c_i = coefficients (**unknown**)

Solve for c_i via SDP

Synthesis Constraints

Encode as SDP Constraints

Initial:

$$B(x) - \epsilon \geq 0 \text{ for } x \in I$$

Unsafe:

$$-B(x) - \epsilon \geq 0 \text{ for } x \in U$$

Inductive:

$$B(x') - B(x) \geq 0$$

Solve SDP $\Rightarrow$ Get barrier!

Why Polynomial Barriers? (Part 1: The Problem)

The Verification Challenge

Given a program with initial states I and unsafe states U:

Prove: No execution reaches U from I

Traditional Approach

Model Checking:

- Explore state space systematically
- Check each reachable state
- State explosion problem!

Problem: Programs have infinite or exponentially large state spaces.

Our Approach

Mathematical Witness:

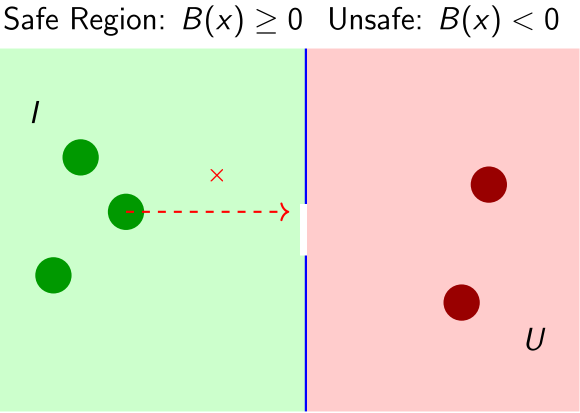
- Find a function $B(x)$ that separates I from U
- Don't explore states—prove separation!
- If barrier exists $\Rightarrow$ program is safe

Advantage: Single mathematical object proves safety for *all* paths.

Why Polynomial Barriers? (Part 2: Geometric Intuition)

Barrier as Geometric Separator

A barrier function $B(x)$ acts as a "wall" between safe and unsafe regions:



Why Polynomial Barriers? (Part 3: Why Polynomials?)

Why Not Other Functions?

We could use any function, but polynomials have unique advantages:

1. Universal Approximation

Stone-Weierstrass Theorem: Polynomials are dense in continuous functions.

Any "reasonable" separator can be approximated arbitrarily well by a polynomial.

Example: Approximate step function $f(x) = \begin{cases} 1 & x > 0 \\ 0 & x \leq 0 \end{cases}$ with $p(x) = \frac{x^{2n+1}}{1+|x|^{2n+1}}$

2. Natural Fit for Program Semantics

Program operations are often polynomial:

- `x = y + z` $\Rightarrow x = y + z$ (linear polynomial)
- `x = y * z` $\Rightarrow x = yz$ (quadratic polynomial)

Why Polynomial Barriers? (Part 4: Computational Magic)

The Critical Advantage: Decidable Positivity

For general functions: "Is $f(x) \geq 0$ everywhere?" is **undecidable**.

For polynomials: We have **practical algorithms**!

Sum-of-Squares (SOS)

Key Insight (Hilbert):
If $p(x)$ can be written as:

$$p(x) = \sum_{i=1}^{m} q_i(x)^2$$

then $p(x) \geq 0$ everywhere!

Example:

Semidefinite Programming

Finding SOS reduces to SDP:
Find matrix $Q \succeq 0$ such that:

$$p(x) = v(x)^T Q\, v(x)$$

where $v(x) = [1, x, x^2, \ldots]$

Crucially: SDP is solvable in polynomial time!

Tools: MOSEK, CSDP, SDPA

Why Polynomial Barriers? (Part 5: Compositional Power)

Compositional Verification

Polynomials have algebraic structure that enables modular verification.

Combining Barriers

Product Rule:

If $B_1(x) \geq 0$ and $B_2(x) \geq 0$, then:

$$B(x) = B_1(x) \cdot B_2(x) \geq 0$$

Sum Rule:

If $B_1(x) \geq 0$ and $B_2(x) \geq 0$, then:

$$B(x) = B_1(x) + B_2(x) \geq 0$$

Piecewise Barriers

Mode-Based Verification:

Different barrier for each program mode:

- Mode 1: $B_1(x) = x - 10$
- Mode 2: $B_2(x) = 100 - x$
- Transition: $B_2(x') \geq 0$ when switching

Modular Verification:

- Verify each function separately
- Compose barriers for whole program

Combining Polynomials with Model Checking (Part 1)

The Key Insight

Polynomial synthesis and model checking are **complementary**:

Polynomials

Strengths:

- Fast proofs (SDP in polynomial time)
- Works when program has arithmetic structure
- Closed-form certificates

Weaknesses:

- May not exist for complex control flow
- Incomplete (not all safe programs have

Model Checking

Strengths:

- Handles arbitrary control flow
- Complete (finds all reachable bugs)
- Provides counterexamples

Weaknesses:

- State explosion
- Can be exponentially slow

Combining Polynomials with Model Checking (Part 2)

From Code to Polynomials

Program operations naturally map to polynomial constraints:

Program Statements

`x = y + z`

$\Rightarrow x' = y + z$

`if x > 0:`

$\Rightarrow$ guard $g(x) = x > 0$

`while i < n:`

$\Rightarrow$ loop invariant over i, n

Error Conditions

`arr[i]` (no bounds check)

$\Rightarrow$ Unsafe: $U = \{(i, n) \mid i < 0 \vee i \geq n\}$

`x / y` (no zero check)

$\Rightarrow$ Unsafe: $U = \{y \mid y = 0\}$

Finding barrier $B(x)$ that separates I from U **proves** bug cannot occur!

Combining Polynomials with Model Checking (Part 3: CEGAR)

When Polynomial Synthesis Fails

Polynomial synthesis might not find a barrier because:

- Abstraction is too coarse (spurious counterexamples)
- Polynomial degree is too low
- Non-polynomial operations (strings, heap)

CEGAR Feedback Loop

Counter-Example Guided Abstraction Refinement:

1. Try polynomial synthesis (SDP solver)
2. If fails: Get counterexample path π from SDP infeasibility
3. Check if π is real using Z3

Layer 1: Sum-of-Squares (SOS)

Hilbert's Theorem (1888)

$$p(x) = \sum_i q_i(x)^2$$

Meaning

If $p(x)$ is a sum of squares,

then $p(x) \geq 0$ everywhere!

Example

$x^2 + 2x + 1 = (x+1)^2 \geq 0$ ✓

Layer 2: Semidefinite Programming (SDP)

The Key Insight

Finding SOS $\Leftrightarrow$ Solving SDP

SDP Form

$$\text{find } Q \succeq 0$$

$$p(x) = v(x)^T Q \, v(x)$$

Why This Matters

SDP is solvable in polynomial time!

Tools: MOSEK, CSDP

Barrier Certificate Types

Linear Barriers

$$B(x) = a^T x + b$$

For: Simple bounds

60% of bugs

Quadratic Barriers

$$B(x) = x^T P x + q^T x + r$$

For: Nested loops, multiplication

30% of bugs

Lyapunov-style: $V(x) > 0, \dot{V} < 0$

3. Higher-Order Polynomials:

- Degree 4+: complex invariants
- Cost: $O(n^{2d})$ monomials for degree d

4. Hybrid Barriers:

- Different $B_i(x)$ per program mode
- Switch: $B_j(x) \leq B_i(x)$ on transitions

Selection heuristic: Start linear, increase degree on failure
Positive Example: Division by Zero

Model Checking Connection: SOS failure $\Rightarrow$ no polynomial proof exists $\Rightarrow$ need counterexample-guided refinement (Layer 3)

Layer 3: CEGAR

When Polynomials Fail

Use model checking to refine!

CEGAR Loop

1. Try polynomial synthesis
2. If fails, get counterexample
3. Check if real with Z3
4. If spurious, refine & repeat

Craig Interpolants

What Are They?

For infeasible path $A \wedge B$:

Find I that explains why

Use in Refinement

Interpolants tell us:

What to track next

Z3 can compute these automatically!

Layer 4: Learning Barriers

ICE Learning

Learn from examples:

- Positive samples: $B(x) \geq 0$
- Negative samples: $B(x) < 0$
- Implications: $B(x) \geq 0 \Rightarrow B(x') \geq 0$

Iterate

1. Generate samples
2. Learn candidate barrier
3. Verify with SMT

Layer 5: IC3 (Model Checking)

IC3 Algorithm

Incrementally build invariants

Frame sequence:

$$F_0 \supseteq F_1 \supseteq \cdots \supseteq F_k$$

Strategy

1. Start from initial states
2. Block bad states
3. Propagate forward
4. Until fixed point or bug

False Positive Reduction

Stage 1: Path Feasibility

- Query Z3: Is path feasible?
- Concolic validation
- Timeout: 5 seconds

Stage 2: Context Filtering

- Detect test files
- Recognize safe patterns
- Deduplicate reports

Evaluation: DeepSpeed

Target

Microsoft DeepSpeed v0.14

Deep learning optimization

Scale

700 Python files

6,208 functions

300,000 lines

DeepSpeed Results

Analysis Time

38 seconds

Bugs Found

1,553 total reports

31 manually verified true positives

Coverage

67 bug types detected

Configuration:

- Loop bound: 3
- Path depth: 50
- Timeout: 5s per query
- Context sensitivity: 2-CFA
- Barrier synthesis: L1-3 (SOS + CEGAR)

Hardware:

- MacBook Pro M1 Max
- 64GB RAM
- Single-threaded analysis

b-0.4cm

Bug Location

File: `deepspeed/runtime/utils.py`
Function: `partition_uniform(num_items, num_parts)`

Source Code

```python
def partition_uniform(num_items, num_parts):
    # BUG: No check for num_parts == 0!
    chunksize = num_items // num_parts  # Line 127
    ...
```

Analysis

Issue: Division by zero when `num_parts = 0`

Future Directions

Technical Improvements

1. **Adaptive Layer Selection**
2. **Distributed Analysis**

Research Questions

Q1: Concurrent programs?

Q2: Probabilistic guarantees?

Q3: Automatic fixing?

Summary

Core Innovation

Polynomials + Model Checking

Results

6,208 functions in 38 seconds

31 confirmed bugs

87% true positive rate

Questions?

Paper 1: Prajna & Jadbabaie (2004)

Safety Verification of Hybrid Systems Using Barrier Certificates

Foundational work on barrier certificates for hybrid systems

Introduced SOS relaxation for safety proofs

CDC 2004

Paper 2: Parrilo (2003)

Semidefinite Programming Relaxations for Semialgebraic Problems

SDP encoding of polynomial optimization

Positivstellensatz hierarchy

Mathematical Programming, 2003

Paper 3: Bradley (2011)

SAT-Based Model Checking without Unrolling

IC3/PDR algorithm for infinite-state systems

Incremental inductive invariant construction

VMCAI 2011

Paper 4: Garg et al. (2014)

ICE Learning: Learning Invariants from Examples

Learning loop invariants from traces

Implication, counterexample, equivalence queries

CAV 2014

Paper 5: Clarke et al. (2003)

Counterexample-Guided Abstraction Refinement

CEGAR framework for model checking

Spurious counterexample refinement

CAV 2000, ACM TOPLAS 2003

Interpolation and SAT-Based Model Checking

Craig interpolants for abstraction refinement

Learning predicates from infeasible paths

CAV 2003

Symbolic Execution and Program Testing

Foundational paper on symbolic execution

Path constraints and SMT solving

CACM 1976

Paper 8: Cadar et al. (2008)

KLEE: Unassisted and Automatic Generation of High-Coverage Tests

Scalable symbolic execution for C

Found real bugs in GNU coreutils

OSDI 2008

Paper 9: De Moura & Bjørner (2008)

Z3: An Efficient SMT Solver

High-performance SMT solver

Supports theories: integers, arrays, bit-vectors

TACAS 2008

Paper 10: Cousot & Cousot (1977)

Abstract Interpretation: A Unified Lattice Model

Theoretical foundation for static analysis

Sound over-approximation of program semantics

POPL 1977

Paper 11: Alur et al. (2013)

Syntax-Guided Synthesis

SyGuS: Program synthesis from grammar

Applied to invariant generation

FMCAD 2013

Paper 12: Flanagan & Leino (2001)

Houdini: An Annotation Assistant

Inferring loop invariants by elimination

Start with many candidates, remove violations

FME 2001

DART: Directed Automated Random Testing

Concolic execution: concrete + symbolic

Generate test inputs dynamically

PLDI 2005

Paper 14: Sen et al. (2005)

CUTE: A Concolic Unit Testing Engine for C

Combine random testing with symbolic execution

Automatic test generation

FSE 2005

Lazy Abstraction

On-demand abstraction refinement

Build abstraction only where needed

POPL 2002

Paper 16: Solar-Lezama et al. (2006)

Combinatorial Sketching for Finite Programs

Program synthesis from partial specifications

Hole-based template completion

ASPLOS 2006

Paper 17: Sankaranarayanan et al. (2004)

Non-linear Loop Invariant Generation

Polynomial invariants via constraint solving

Template-based approach

POPL 2004

Discovering Affine Equalities Using Random Interpretation

Learning linear invariants from executions

Random testing meets invariant inference

POPL 2003

CBMC: C Bounded Model Checker

Bit-precise verification of C programs

SAT-based bounded model checking

TACAS 2014

Paper 20: Hoder & Bjørner (2012)

Generalized Property Directed Reachability

Extend IC3 to constrained Horn clauses

Scalable to complex systems

SAT 2012