Al-based Blackbox Code Deobfuscation
Understand, Improve and Mitigate

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ABSTRACT
Code obfuscation aims at protecting Intellectual Property and other secrets embedded into software from being retrieved. Recent works leverage advances in artificial intelligence with the hope of getting blackbox deobfuscators completely immune to standard (whitebox) protection mechanisms. While promising, this new field of AI-based blackbox deobfuscation is still in its infancy. In this article we deepen the state of AI-based blackbox deobfuscation in three key directions: understand the current state-of-the-art, improve over it and design dedicated protection mechanisms. In particular, we define a novel generic framework for AI-based blackbox deobfuscation encompassing prior work and highlighting key components; we are the first to point out that the search space underlying code deobfuscation is too unstable for simulation-based methods (e.g., Monte Carlo Tree Search used in prior work) and advocate the use of robust methods such as S-metaheuristics; we propose the new optimized AI-based blackbox deobfuscator Xyntia which significantly outperforms prior work in terms of success rate (especially with small time budget) while being completely immune to the most recent anti-analysis code obfuscation methods; and finally we propose two novel protections against AI-based blackbox deobfuscation, allowing to counter Xyntia’s powerful attacks.

KEYWORDS
Binary-level code analysis, deobfuscation, artificial intelligence

1 INTRODUCTION
Context. Software contain valuable assets, such as secret algorithms, business logic or cryptographic keys, that attackers may try to retrieve. The so-called Man-At-The-End-Attacks scenario (MATE) considers the case where software users themselves are adversarial and try to extract such information from the code. Code obfuscation [12, 13] aims at protecting codes against such attacks, by transforming a sensitive program \( P \) into a functionally equivalent program \( P' \) that is more “difficult” (more expensive, for example, in money or time) to understand or modify. On the flip side, code deobfuscation aims to extract information from obfuscated codes.

Whitebox deobfuscation techniques, based on advanced symbolic program analysis, have proven extremely powerful against standard obfuscation schemes [3, 5, 10, 22, 29, 31, 37] – especially in local attack scenarios where the attacker analyses pre-identified parts of the code (e.g., trigger conditions). But they are inherently sensitive to the syntactic complexity of the code under analysis, leading to recent and effective countermeasures [12, 26, 27, 38].

AI-based blackbox deobfuscation. Despite being rarely sound or complete, artificial intelligence (AI) techniques are flexible and often provide good enough solutions to hard problems in reasonable time. They have been therefore recently applied to binary-level code deobfuscation. The pioneering work by Blazytko et al. [7] shows how Monte Carlo Tree Search (MCTS) [9] can be leveraged to solve local deobfuscation tasks by learning the semantics of pieces of protected codes in a blackbox manner, in principle immune to the syntactic complexity of these codes. Their method and prototype, Syntia, have been successfully used to reverse state-of-the-art protectors like VMProtect [35], Themida [28] and Tigrress [11], drawing attention from the software security community [8].

Problem. While promising, AI-based blackbox (code) deobfuscation techniques are still not well understood. Several key questions of practical relevance (e.g., deobfuscation correctness and quality, sensitivity to time budget) are not addressed in Blazytko et al.’s original paper, making it hard to exactly assess the strengths and weaknesses of the approach. Moreover, as Syntia comes with many hard-coded design and implementation choices, it is legitimate to ask whether other choices lead to better performance, and to get a broader view of AI-based blackbox deobfuscation methods. Finally, it is unclear how these methods compare with recent proposals for greybox deobfuscation [16] or general program synthesis [6, 30], and how to protect from such blackbox attacks.

Goal. We focus on advancing the current state of AI-based blackbox deobfuscation methods in the following three key directions: (1) generalize the initial Syntia proposal and refine the initial experiments by Blazytko et al. in order to better understand AI-based blackbox methods, (2) improve the current state-of-the-art (Syntia) through a careful formalization and exploration of the design space and evaluate the approach against greybox and program synthesis methods, and finally (3) study how to mitigate such AI-based attacks. Especially, we study the underlying search space, bringing new insights for efficient blackbox deobfuscation, and promote the application of S-metaheuristics [33] instead of MCTS.
Contributions. Our main contributions are the following:

- We refine experiments by Blazytko et al. in a systematic way, highlighting both new strengths and new weaknesses of the initial Syntia proposal for AI-based blackbox deobfuscation (Section 4). Especially, Syntia (based on Monte Carlo Search Tree, MCTS) is far less efficient than expected for small time budget (its typical usage scenario) and lacks robustness;
- We propose a missing formalization of blackbox deobfuscation (Section 4) and dig into Syntia internals to rationalize our observations (Section 4.4). It appears that the search space underlying blackbox code deobfuscation is too unstable to rely on MCTS – especially assigning a score to a partial node through simulation leaves here to poor estimations. As a result, Syntia is here almost enumerative;
- We propose to see (Section 5) blackbox deobfuscation as an optimization problem rather than a single player game, allowing to reuse S-metaheuristics [33], known to be more robust than MCTS on unstable search space (especially, they do not need to score partial states). We propose Xyntia (Section 5), an AI-based blackbox deobfuscator using Iterated Local Search (ILS) [24], known among S-metaheuristics for its robustness. Thorough experiments show that Xyntia keeps the benefits of Syntia while correcting most of its flaws. Especially, Xyntia significantly outperforms Syntia, synthesizing twice more expressions with a budget of 1s/expr than Syntia with 600s/expr. Other meta-heuristics also clearly beat MCTS, even if they are less effective here than ILS;
- We evaluate Xyntia against other state-of-the-art attackers (Section 6), namely the QSynth greybox deobfuscator [16], program synthesizers (CVC4 [6] and STOKE [30]) and pattern-matching based simplifiers. Xyntia outperforms all of them – it finds 2× more expressions and is 30× faster than QSynth on heavy protections;
- We evaluate Xyntia against state-of-the-art defenses (Section 7), especially recent anti-analysis proposals [14, 26, 32, 36, 38]. As expected, Xyntia is immune to such defenses. In particular, it successfully bypasses side-channels [32], path explosion [26] and MBA [38]. We also use it to synthesizes VM-handlers from state-of-the-art virtualizers [11, 35, 36];
- Finally, we propose the two first protections against AI-based blackbox deobfuscation (Section 8). We observe that all phases of blackbox techniques can be thwarted (hypothesis, sampling and learning) and propose two practical methods exploiting these limitations, and discuss them in the context of virtualization-based obfuscation: (1) semantically complex handlers; (2) merged handlers with branch-less conditions. Experiments show that both protections are highly effective against blackbox attacks.

We hope that our results will help better understand AI-based code deobfuscation, and lead to further progress in this promising field.

Availability. Benchmarks and code are available online. Also, we put a fair amount of experimental data in appendices for convenience. While the core paper can be read without, this material will still be made available online in a technical report.

2 BACKGROUND

2.1 Obfuscation

Program obfuscation [12, 13] is a family of methods designed to make reverse engineering (understanding programs’ internals) hard. It is employed by manufacturers to protect intellectual property and by malware authors to hinder analysis. It transforms a program P in a functionally equivalent, more complex program P’ with an acceptable performance penalty. Obfuscation does not ensure that a program cannot be understood – this is impossible in the MATE context – but aims to delay the analysis as much as possible in order to make it unprofitable. Thus, it is especially important to protect from automated deobfuscation analyses (anti-analysis obfuscation). We present here two important obfuscation methods.

Mixed Boolean-Arithmetic (MBA) encoding [38] transforms an arithmetic and/or Boolean expression into an equivalent one, combining arithmetic and Boolean operations. It can be applied iteratively to increase the syntactic complexity of the expression. Eyrolles et al. [18] shows that SMT solvers struggle to answer equivalence requests on MBA expressions, preventing the automated simplification of protected expressions by symbolic methods.

Virtualization [36] translates an initial code P into a bytecode B together with a custom virtual machine. Execution of the obfuscated code can be divided in 3 steps (Fig. 1): (1) fetch the next bytecode instruction to execute, (2) decode the bytecode and finds the corresponding handler, and finally execute the handler. Virtualization hides the real control-flow-graph (CFG) of P, and reversing the handlers is key for reversing the VM. Virtualization is notably used in malware [19, 34].

![Virtualization based obfuscation](image)

Figure 1: Virtualization based obfuscation

2.2 Deobfuscation

Deobfuscation aims at reverting an obfuscated program back to a form close enough to the original one, or at least to a more understandable version. Along the previous years, symbolic deobfuscation methods based on advanced program analysis techniques have proven to be very efficient at breaking standard protections [3, 5, 10, 22, 29, 31, 37]. However, very effective countermeasures start to emerge, based on deep limitations of the underlying code-level reasoning mechanisms and potentially strongly limiting their usage [3, 26, 27, 32, 36]. Especially, all such methods are ultimately sensitive to the syntactic complexity of the code under analysis.

2.3 Syntia an AI-based blackbox deobfuscator

Artificial intelligence based blackbox deobfuscation has been recently proposed by Blazytko et al. [7], implemented in the Syntia tool, to learn the semantic of well-delimited code fragments, e.g. MBA expressions or VM handlers. The code under analysis is seen as a blackbox that can only be queried (i.e., executed under chosen
inputs to observe results). Syntia samples input-output (I/O) relations, then use a learning engine to find an expression mapping sampled inputs to their observed outputs. Because it relies on a limited number of samples, results are not guaranteed to be correct. However, being fully blackbox, it is in principle insensitive to syntactic complexity.

**Scope.** Syntia tries to infer a simple semantics of heavily obfuscated local code fragments—e.g., trigger based conditions or VM handlers. Understanding these fragments is critical to fulfill analysis.

**Workflow.** Syntia’s workflow is representative of AI-based black-box deobfuscators. First, it needs (1) a reverse window i.e., a subset of code to work on; (2) the location of its inputs and outputs. Consider the code in Listing 1 evaluating a condition at line 4. To understand this condition, a reverser focuses on the code between lines 1 and 3. This code segment is our reverse window. The reverser then needs to locate relevant inputs and outputs. The condition at line 4 is performed on t3. This is our output. The set of inputs contains any variables (register or memory location at assembly level) influencing the outputs. Here, inputs are x and y. Armed with these information, Syntia samples inputs randomly and observes resulting outputs. In our example, it might consider samples (x → 1, y → 2), (x → 0, y → 1) and (x → 3, y → 4) which respectively evaluate t3 to 3, 1 and 7. Syntia then synthesize an expression matching these observed behaviors, using Monte Carlo Tree Search (MCTS) over the space of all possible (partial) expressions. Here, it rightly infers that t3 = x + y and the reverser concludes that the condition is x + y = 5, where a symbolic method will typically simply retrieve that ((x ∨ 2y) × 2 − (x ⊕ 2y) − y) = 5.

```
1 int t1 = 2 * y;
2 int t2 = x | t1 ;
3 int t3 = t2 * 2 - (x ^ t1) - y ;
4 if (t3 == 5) ...
```

Listing 1: Obfuscated condition

3 MOTIVATION

3.1 Attacker model

In the MATE scenario, the attacker is the software user himself. He has only access to the obfuscated version of the code under analysis and can read or run it at will. We consider that the attacker is highly skilled in reverse engineering but has limited resources in terms of time or money. We see reverse engineering as a human-in-the-loop process where the attacker combines manual analysis with automated state-of-the-art deobfuscation methods (slicing, symbolic execution, etc.) on critical, heavily obfuscated code fragments like VM handlers or trigger-based conditions. Thus, an effective defense strategy is to thwart automated deobfuscation methods.

3.2 Syntactic and semantic complexity

We now intuitively motivate the use of blackbox deobfuscation. Consider that we reverse a software protected through virtualization. We need to extract the semantics of all handlers, which usually perform basic operations like \( h(x, y) = x + y \). Understanding \( h \) is trivial, but it can be protected to hinder analysis. Eq. (1) shows how MBA encoding hides \( h \)’s semantics.

\[
h(x, y) = x + y \overset{mba}{\longrightarrow} (x ∨ 2y) × 2 − (x ⊕ 2y) − y \tag{1}
\]

Such encoding syntactically transforms the expression to make it incomprehensible while preserving its semantics. To highlight the difference between syntax and semantics, we distinguish:

(1) **The syntactic complexity** of expression \( e \) is the size of \( e \), i.e. the number of operators used in it;

(2) **The semantic complexity** of expression \( e \) is the smallest size of expressions \( e' \) (in a given language) equivalent to \( e \).

For example, in the MBA language, \( x + y \) is syntactically simpler than \((x ∨ 2y) × 2 − (x ⊕ 2y) − y\), yet they have the same semantic complexity as they are equivalent. Conversely, \( x + y \) is more syntactically complex than \((x + y) ∧ 0\), which equals 0. We do not claim to give a definitive definition of semantic and syntactic complexity—as smaller is not always simpler—but introduce the idea that two kinds of complexity exist and are independent.

The encoding in Eq. (1) is simple, but it can be repeatedly applied to create a more syntactically complex expression, leading the reverser to either give up or try to simplify it automatically. Whitebox methods based on symbolic execution (SE) [29, 37] and formula simplifications (in the vein of compiler optimizations) can extract the semantic of an expression, yet they are sensitive to syntactic complexity and will not return simple versions of highly obfuscated expressions. Conversely, blackbox deobfuscation treats the code as a blackbox, considering only sampled I/O behaviors. Thus increasing syntactic complexity, as usual state-of-the-art protections do, has simply no impact on blackbox methods.

3.3 Blackbox deobfuscation in practice

We now present how blackbox methods integrate in a global deobfuscation process and highlight crucial properties they must hold.

**Global workflow.** Reverse engineering can be fully automated, or handmade by a reverser, leveraging tools to automate specific tasks. While the deobfuscation process operates on the whole obfuscated binary, blackbox modules can be used to analyze parts of the code like conditions or VM handlers. Upon meeting a complex code fragment, the blackbox deobfuscator is called to retrieve a simple semantic expression. After synthesis succeeds, the inferred expression is used to help continue the analysis.

**Requirements.** In virtualization based obfuscation, the blackbox module is typically queried on all VM handlers [7]. As the number of handlers can be arbitrarily high, blackbox methods need to be fast. In addition, inferred expressions should ideally be as simple as the original non-obfuscated expression and semantically equivalent to the obfuscated expression (i.e. correct). Finally, robustness (i.e. the capacity to synthesize complex expressions) is needed to be usable in various situations. Thus, speed, simplicity, correctness, and robustness, are required for efficient blackbox deobfuscation.

4 UNDERSTAND AI-BASED DEOBFUSCATION

We propose a general view of AI-based code deobfuscation fitting state-of-the-art solutions [7, 16]. We also extend the evaluation of Syntia by Blazytko et al. [7], highlighting both some previously unreported weaknesses and strengths. From that we derive general
lessons on the (in)adequacy of MCTS for code deobfuscation, that will guide our new approach (Section 5).

4.1 Problem at hand

AI-based deobfuscation takes an obfuscated expression and tries to infer an equivalent one with lower syntactic complexity. Such problem can be stated as following:

Deobfuscation. Let $e$, $obf$ be 2 equivalent expressions such that $obf$ is an obfuscated version of $e$ – note that $obf$ is possibly much larger than $e$. Deobfuscation aims to infer an expression $e'$ equivalent to $obf$ (and $e$), but with size similar to $e$. Such problem can be approached in three ways depending on the amount of information given to the analyzer:

Blackbox We can only run $obf$. The search is thus driven by sampled I/O behaviors. Syntia [7] is a blackbox approach;

Greybox Here $obf$ is executable and readable but the semantics of its operators is mostly unknown. The search is driven by previously sampled I/O behaviors which can be applied to subparts of $obf$. QSynth [16] is a greybox solution;

Whitebox The analyzer has full access to $obf$ (run, read) and the semantics of its operators is precisely known. Thus, the search can profit from advanced pattern matching and symbolic strategies. Standard static analysis falls in this category.

Blackbox methods. AI-based blackbox deobfuscators follow the framework given in Algorithm 1. In order to deobfuscate code, one must detail a sampling strategy (i.e., how inputs are generated), a learning strategy (i.e., how to learn an expression mapping sampled inputs to observed outputs) and a simplification postprocess. For example, Syntia samples inputs randomly, uses Monte Carlo Tree Search (MCTS) [9] as learning strategy and leverages the Z3 SMT solver [17] for simplification. The choice of the sampling and learning strategies is critical. For example, too few samples could lead to incorrect results while too many could impact the search efficiency, and an inappropriate learning algorithm could impact robustness or speed.

Let us now turn to discussing Syntia’s learning strategy. We show that using MCTS leads to disappointing performances and give insight to understand why.

Algorithm 1: AI-based blackbox deobfuscation framework

| Inputs: |
|---|
| Code : code to analyze |
| Sample : sampling strategy |
| Learn : learning strategy |
| Simplify : expression simulator |

| Output: learned expression or Failure |
|---|
| 1: procedure DEOBFUSCATE(Code, Sample, Learn) |
| 2: Oracle ← Sample(Code) |
| 3: succ, expr ← Learn(Oracle) |
| 4: if succ = True then return Simplify(expr) |
| 5: else return Failure |

4.2 Evaluation of Syntia

We extend Syntia’s evaluation and tackle the following questions left unaddressed by Blazytko et al. [7].

| RQ1 | Are results stable across different runs? |
|---|---|
| This is desirable due to the stochastic nature of MCTS; |

| RQ2 | Is Syntia fast, robust and does it infer simple and correct results? |
|---|---|
| Syntia offers a priori no guarantee of correctness nor quality. Also, we consider small time budget (1s), adapted to human-in-the-loop reverse scenarios but absent from the initial evaluation; |

| RQ3 | How is synthesis impacted by the set of operators’ size? |
|---|---|
| Syntia learns expressions over a search space fixed by predefined grammars. Intuitively, the more operators in the grammar, the harder it will be to converge to a solution. We use 3 sets of operators to assess this impact. |

4.2.1 Experimental setup. We distinguish the success rate (number of expressions inferred) from the equivalence rate (number of expressions inferred and equivalent to the original one). The equivalence rate relies on the Z3 SMT solver [17] with a timeout of 10s. Since Z3 timeouts are inconclusive answers, we define a notion of equivalence range: its lower bound is the proven equivalence rate (number of expression proven to be equivalent) while its upper bound is the optimistic equivalence rate (expressions not proven different, i.e., optimistic = proven + timeout). The equivalence rate is within the equivalence range, while the success rate is higher than the optimistic equivalence rate. Finally, we define the quality of an expression as the ratio between the number of operators in recovered and target expressions. It estimates the syntactic complexity of inferred expressions compared to the original ones. A quality of 1 indicates that the recovered expression has the same size as the target one.

**Benchmarks.** We consider two benchmark suites: B1 and B2. B1² comes from Blazytko et al. [7] and was used to evaluate Syntia. It comprises 500 randomly generated expressions with up to 3 arguments, and simple semantics. It aims at representing state-of-the-art VM-based obfuscators. However, we found that B1 suffers from several significant issues: (1) it is not well distributed over the number of inputs and expression types, making it unsuitable for fine-grained analysis; (2) only 216 expressions are unique modulo renaming – the other 284 expressions are $a$-equivalent, like $x+y$ and $a+b$. These problems threaten the validity of the evaluation.

We thus propose a new benchmark B2 consisting of 1,110 randomly generated expressions, better distributed according to number of inputs and nature of operators – see Appendix A.2 for details. We use three categories of expressions: Boolean, Arithmetic and Mixed Boolean-Arithmetic, with 2 to 6 inputs. Each expression has an Abstract Syntax Tree (AST) of maximal height 3. As a result, B2 is more challenging than B1 and enables a finer-grained evaluation.

**Operator sets.** Table 1 introduces three operator sets: Full, Expr and MBA. We use these to evaluate sensitivity to the search space and answer RQ3. Expr is as expressive as Full even if Expr < Full. MBA can only express Mixed Boolean-Arithmetic expressions [38].

**Configuration.** We run all our experiments on a machine with 6 Intel Xeon E-2176M CPUs and 32 GB of RAM. We evaluate Syntia in its original configuration [7]: the SA-UCT constant is 1.5, we use

²https://github.com/RUB-SySc/syntia/tree/master/samples/mba/tigress
Table 1: Sets of operators

| FULL | {−1, ¬, +, −, ×, ∨, ∧, ⋄, ⊤, ⊥, %, %u, #} |
| EXPR | {−1, ¬, +, −, ×, ∨, ∧, ⋄, ⊤, ⊥, %, %u, #} |
| MFA | {−1, ¬, +, −, ×, ∨, ∧, ⋄} |

50 I/O samples and a maximum playout depth of 0. It also limits Syntia to 50,000 iterations per sample, corresponding to a timeout of 60 s per sample on our test machine.

4.2.2 Evaluation Results. Let us summarize here the outcome of our experiments — see Appendix A.1 for complete results.

RQ1. Over 15 runs, Syntia finds between 362 and 376 expressions of B1 i.e., 14 expressions of difference (2.8% of B1). Over B2, it finds between 349 and 383 expressions i.e., 34 expressions of difference (3.06% of B2). Hence, Syntia is very stable across executions.

RQ2. Syntia cannot efficiently infer B2 (≈ 34% success rate). Moreover, Table 2 shows Syntia to be highly sensitive to time budget. More precisely, with a time budget of 1s/expr, Syntia only retrieves 16.3% of B2. Still, even with a timeout of 600 s/expr, it tops at 42% of B2. In addition, Syntia is unable to synthesize expressions with more than 3 inputs − success rates for 4, 5 and 6 inputs respectively falls to 10%, 2.2% and 1.1%. It also struggles over expressions using a mix of boolean and arithmetic operators, synthesizing only 21%. Still, Syntia performs well regarding quality and correctness. On average, its quality is around 0.60 (for a timeout of 60s/expr i.e., resulting expressions are simpler than the original (non-obfuscated) ones, and it rarely returns non-equivalent expressions − between 0.5% and 0.8% of B2. We thus conclude that Syntia is stable and returns correct and simple results. Yet, it is not efficient enough (solve only few expressions on B2, heavily impacted by time budget) and not robust (number of inputs and expression’s type).

Table 2: Syntia depending on the timeout per expression (B2)

| Succ. Rate | 10s | 60s | 600s |
|-----------|-----|-----|------|
| Equiv. Range | 16.5% | 25.6% | 34.5% | 42.3% |
| Mean Qual | 0.35 | 0.49 | 0.59 | 0.67 |

RQ3. Default Syntia synthesizes expressions over the FULL set of operators. To evaluate its sensitivity to the search space we run it over FULL, EXPR and MFA. Smaller sets do exhibit higher success rates (42% on MFA) but results remain disappointing. Syntia is sensitive to the size of the operator set but is inefficient even with MFA.

Conclusion. Syntia is stable, correct and returns simple results. Yet, it is heavily impacted by the time budget and lacks robustness. It thus fails to meet the requirements given in Section 3.3.

4.3 Optimal Syntia

To ensure the conclusions given in Section 4.4 apply to MCTS and not only to Syntia, we study Syntia extensively to find better set ups (Appendix A.1) for the following parameters: simulation depth, SA-UCT value (configuring the balance between exploitative and explorative behaviors), number of I/O samples and distance. Optimizing Syntia’s parameters slightly improves its results which stay disappointing (at best, ≈ 50% of success rate on MFA in 60 s/expr).

Conclusion. By default, Syntia is well configured. Changing its parameters lead in the best scenario to marginal improvement, hence the pitfalls highlighted seem to be inherent to the MCTS approach.

4.4 MCTS for deobfuscation

Let us explore whether these issues are related to MCTS.

Monte Carlo Tree Search. MCTS creates here a search tree where each node is an expression which can be terminal (e.g. a + 1, where a is a variable) or partial (e.g. U + a, where U is a non-terminal symbol). The goal of MCTS is to expand the search tree smartly, focusing on most pertinent nodes first. Evaluating the pertinence of a terminal node is done by sampling (computing here a distance between the evaluation of sampled input over the node expression against their expected output values). For partial nodes, MCTS relies on simulation: random rules of the grammar are applied to the expression (e.g., U + a ∼ b + a) until it becomes terminal and is evaluated. As an example, let \{(a → 1, b → 0), (a → 0, b → 1)\} be the sampled inputs. The expression b+a (simulated from U+a) evaluates them to (1, 1). If the ground-truth outputs are 1 and −1, the distance will equal δ(1,1) + δ(1,−1) where δ is a chosen distance function. We call the result the pertinence measure. The closer it is to 0, the more pertinent the node U+a is considered and the more the search will focus on it.

Analysis. This simulation-based pertinence estimation is not reliable in our code deobfuscation setting.

- We present in Fig. 2, for different non-terminal nodes, the distance values computed through simulations. We observe that from a starting node, a random simulation can return drastically different results. It shows that the search space is very unstable and that relying on a simulation is misleading (especially in our context where time budget is small);
- Moreover, our experiments show that in practice Syntia is not guided by simulations and behaves almost as if it were an enumerative (BFS) search – MCTS where simulation is non informative. As an example, Fig. 3 compares how the distance evolves over time for Syntia and a custom, fully enumerative, MCTS synthesizer: both are very similar;
- Finally, on B2 with a timeout of 60 s/expr, only 34/341 successfully synthesized expressions are the children of previously most promising nodes. It shows that Syntia successfully synthesized expressions due to its exploratory (i.e., enumerative) behavior rather than to the selection of nodes according to their pertinence.

Conclusion. The search space from blackbox code deobfuscation is too unstable, making MCTS’s simulations unreliable. MCTS in that setting is then almost enumerative and ineffective. That is why Syntia is slow and not robust, but returns simple expressions.

4.5 Conclusion

While Syntia returns simple results, it only synthesizes semantically simple expressions and is slow. These unsatisfactory results can be explained by the fact that the search space is too unstable, making the use of MCTS unsuitable. In the next section, we show that methods avoiding the manipulating of partial expressions (and thus free from simulation) are better suited to deobfuscation.
We define a new AI-based blackbox deobfuscator, dubbed Xyntia a, and can be modeled as an optimization problem. The objective is to synthesize an expression from inputs-outputs samples that can generate multiple terminal ones through simulations, leading to completely different results.

**5 IMPROVE AI-BASED DEOBFUSCATION**

We define a new AI-based blackbox deobfuscator, dubbed Xyntia, leveraging S-metaheuristics [33] and Iterated Local Search (ILS) [24] and compare its design to rival deobfuscators. Unlike MCTS, S-metaheuristics only manipulate terminal expressions and do not create tree searches, thus we expect them to be better suited than MCTS for code deobfuscation. Among S-metaheuristics, ILS is particularly designed for unstable search spaces, with the ability to remember the last best solution encountered and restart the search from that point. We show that these methods are well-guided by the distance function and significantly outperform MCTS in the context of blackbox code deobfuscation.

### 5.1 Deobfuscation as Optimization

As presented in Section 4, Syntia frames deobfuscation as a single player game. We instead propose to frame it as an optimization problem using ILS as learning strategy.

**Blackbox deobfuscation: an optimization problem.** Blackbox deobfuscation synthesizes an expression from inputs-outputs samples and can be modeled as an optimization problem. The objective function, noted \( f \), measures the similarity between current and ground truth behaviors by computing the sum of the distances between found and objective outputs. The goal is to infer an expression minimizing the objective function over the I/O samples. If the underlying grammar is expressive enough, a minimum exists and matches all sampled inputs to objective outputs, zeroing \( f \). The reliability of the found solution depends on the number of I/O samples considered. Too few samples would not restrain search enough and lead to flawed results.

**Solving through search heuristics.** S-metaheuristics [33] can be advantageously used to solve such optimization problems. A wide range of heuristics exists (Hill Climbing, Random Walk, Simulated Annealing, etc.). They all iteratively improve a candidate solution by testing its “neighbors” and moving along the search space. Because solution improvement is evaluated by the objective function, it is said to guide the search.

**Iterated Local Search.** Some S-metaheuristics are prone to be stuck in local optimums so that the result depends on the initial input chosen. Iterated Local Search (ILS) [24] tackles the problem through iteration of search and the ability to restart from previously seen best solutions. Note that ILS is parameterized by another search heuristics (for us: Hill Climbing). Once a local optimum is found by this side search, ILS perturbs it and uses the perturbed solution as initial state for the side search. At each iteration, ILS also saves the best solution found. Unlike most other S-metaheuristics (Hill Climbing, Random Walk, Metropolis Hastings and Simulated Annealing, etc.), if the search follows a misleading path, ILS can restore the best seen solution so far to restart from an healthy state.

### 5.2 Xyntia’s internals

Xyntia is built upon 4 components: the optimization problem we aim to solve, the oracle which extracts the sampling information from the protected code under analysis and the search heuristics.

**Oracle.** The oracle is defined by the sampling strategy which depicts how the protected program must be sampled and how many samples are considered. As default, we consider that our oracle samples 100 inputs over the range \([-50;49]\). Five are not randomly generated but equal interesting constant vectors \((0, 1, -1, \min_s, \max_s)\). These choices arise from a systematic study of the different settings to find the best design (see Appendix A.2.2).

**Optimization problem.** The optimization problem is defined as follows. The search space is the set of expressions expressible using the \( \text{EXPR} \) set of operators (see Table 1), and considers a unique constant 1. This grammar enables Xyntia to reach optimal results while being as expressive as rivals’ tools like Syntia [7]. Besides, we consider the objective function:

\[
f_{\text{opt}}(\delta) = \sum_i \log_2(1 + |o_i - o^*_i|)
\]

It computes the Log-arithmetic distance between synthesized expressions’ outputs (\( \delta \)) and sampled ones (\( \delta^* \)). The choice of the grammar and of the objective function are respectively discussed in Section 5.3 and Appendix A.2.2.

**Search.** Xyntia leverages Iterated Local Search (ILS) to minimize our objective function and so to synthesize target expressions. We
present now how ILS is adapted to our context. ILS applies two steps starting from a random terminal (a constant or a variable):

- ILS reuses the best expression found so far to perturb it by randomly selecting a node of the AST and replacing it by a random terminal node. The resulting AST is kept even if the distance increases and passed to the next step.
- Iterative Random Mutations: the side search (in our case Hill Climbing) iteratively mutates the input expression until it cannot improve anymore. We estimate that no more improvement can be done after 100 inconclusive mutations. A mutation (see Fig. 4) consists in replacing a randomly chosen node of the abstract syntax tree (AST) by a leaf or an AST of depth one (only one operator). At each mutation, it keeps the version of the AST minimizing the distance function. During mutations, the best solution so far is updated to be restored in the perturbation step. If a solution nullifies the objective function, it is directly returned.

These two operations are iteratively performed until timeout is out (by default 60 s) or an expression mapping all I/O samples is found. Furthermore, as Syntia applies Z3’s simplifier to “clean up” recovered expressions, we add a custom post-process expression simplifier, applying simple rewrite rules until a fixpoint is reached.

Appendix A.2.2 compares Xyntia with and without simplification. Xyntia is implemented in OCaml [23], within the BINSEC framework for binary-level program analysis [15]. It comprises ≈9k lines of code.

| Random selection | Mutation | Mutated |
|------------------|----------|---------|
| + (-a)            | (b) + (-a) |

Figure 4: Random mutation example

5.3 Xyntia evaluation

We now evaluate Xyntia in depth and compare it to Syntia. As with Syntia we answer the following questions:

RQ4 Are results stable across different runs?

RQ5 Is Xyntia robust, fast and does it infer simple and correct results?

RQ6 How is synthesis impacted by the set of operators’ size?

Configuration. For all our experiments, we default to locally optimal Xyntia (Xyntia_{OPT}) presented in Section 5.2. It learns expressions over Expr, samples 100 inputs (95 randomly and 5 constant vectors) and uses the Log-arithmetic distance as objective function.

Interestingly, all results reported here also hold (to a lesser extend regarding efficiency) for other Xyntia configurations (Section 5.4), especially these versions consistently beat Syntia.

RQ4. Over 15 runs Xyntia always finds all 500 expressions in B1 and between 1051 to 1061 in B2. The difference between the best and the worst case is only 10 expressions (0.9% of B2). Thus, Xyntia is very stable across executions.

RQ5. Unlike Syntia, Xyntia performs well on both B1 and B2 with a timeout of 60 s/expr. Fig. 5 reveals that it is still successful for a timeout of 1 s/expr. (78% proven equivalence rate). Moreover, for a timeout of 600 s/expr. (10 min), Xyntia finds 2× fewer expressions than Syntia with a 1 s/expr. time budget. In addition, Xyntia handles well expressions using up to 5 arguments and all expression types. Its mean quality is around 0.93, which is very good (objective is 1), and it rarely returns not equivalent expressions – only between 1.3% and 4.9%. Thus, Xyntia reaches high success and equivalence rate. It is fast, synthesizing most expressions in ≤ 1s, and it returns simple and correct results.

Figure 5: Equivalence range of Syntia and Xyntia (Xyntia_{OPT}) depending on timeout (B2)

RQ6. Xyntia by default synthesizes expressions over Expr while Syntia infers expressions over FULL. To compare their sensitivity to search space and show that previous results was not due to search space inconsistency, we run Xyntia over FULL, Expr and Mba and compare it to Syntia. Experiments shows that Xyntia reaches high equivalence rates for all operator sets while Syntia results stay low.

Still, Xyntia seems more sensitive to the size of the set of operators than Syntia. Its proven equivalence rate decreases from 90% (Expr) to 71% (FULL) while Syntia decreases only from 38.7% (Expr) to 33.7% (FULL). Conversely, as for Syntia, restricting to Mba benefits to Xyntia. Thus, like Syntia, Xyntia is sensitive to the size of the operator set. Yet, Xyntia reaches high equivalence rates even on FULL while Syntia remains inefficient even on Mba.

Conclusion. Xyntia is a lot faster and more robust than Syntia. It is also stable and returns simple expressions. Thus, Xyntia, unlike Syntia, meets the requirements given in Section 3.3.

5.4 Optimal Xyntia and other S-Metaheuristics

Previous experiments consider the Xyntia_{OPT} configuration of Xyntia. It comes from a systematic evaluation of the design space (Appendix A.2.2). To do so, we considered (1) different S-metaheuristics (Hill Climbing, Random Walk, Simulated Annealing, Metropolis Hastings and Iterated Local Search); (2) different sampling strategies; (3) different objective functions. This evaluation confirms that Xyntia_{OPT} is locally optimal and that ILS, being able to restore best expression seen after a number of unsuccessful mutations, outperforms other S-metaheuristics. Moreover, all S-metaheuristics – except Hill Climbing – outperforms Syntia.

It confirms that estimating non terminal expression’s pertinence through simulations, as MCTS does, is not suitable for deobfuscation (Section 4.4). It is far more relevant to manipulate terminal expressions only as S-metaheuristics.
Conclusion. Principled and systematic evaluation of Xyntia’s design space lead to the locally optimal Xyntia_{Opt} configuration. It notably shows that ILS outperforms other tested S-metaheuristics. Moreover, all these S-metaheuristics – except Hill Climbing – outperform MCTS, confirming that manipulating only terminal expressions is beneficial.

5.5 On the effectiveness of ILS over MCTS

Unlike MCTS, ILS does not generate a search tree and only manipulates terminal expressions. As such, no simulation is performed and the distance function guides the search well. Indeed, as Fig. 6 presents, the distance follows a step-wise progression. Distance evolution is drastically different from Syntia and enumerative MCTS (Fig. 3). It assesses that unlike them, Xyntia is guided by the distance function. This enables Xyntia to synthesize deeper expressions that would be out of reach for enumerative search. Moreover, note that Xyntia globally follows a positive trend i.e. it does not unlearn previous work. Indeed, before each perturbation, the best expression found from now is restored. Thus, if iterative mutations follow a misleading path, the resulting solution is not kept and the best solution is reused to be perturbed. Keeping the current best solution is of first relevance as the search space is highly unstable and enables Xyntia to be more reliable and less dependant of randomness.

![Figure 6: Xyntia (Xyntia_{Opt}): distance evolution](image)

5.6 Limitations

Blackbox methods rely on two main steps, sampling and learning, which both show weaknesses. Indeed, Xyntia and Syntia randomly sample inputs to approximate the semantics of an expression. It then assumes that samples depict all behaviors of the code under analysis. If this assumption is invalid then the learning phase will miss some behaviors, returning partial results. As such, blackbox deobfuscation is not appropriate to handle points-to-functions.

Learning can itself be impacted by other factors. For instance, learning expressions with unexpected constant values is hard. Indeed, the grammar of Xyntia and Syntia only considers constant value 1. Thus, finding expressions with constant values absent from the grammar requires to create them (e.g., encoding 3 as 1 + 1 + 1), which may be unlikely. A naive solution is to add to the grammar additional constant values but it significantly impacts efficiency. Appendix A.2.3 studies the effect of introducing higher numbers of constant values in Xyntia. For 100 values, the equivalence rate is divided by 2 (resp., by 4 for 200 values). Still, Section 7 shows that Xyntia can synthesize interesting constant values (unlike Syntia).

5.7 Conclusion

Because of the high instability of the search space, Iterated Local Search is much more appropriate than MCTS (and, to a lesser extent, than other S-metaheuristics) for blackbox code deobfuscation, as it manipulates terminal expressions only and is able to restore the best solution seen so far in case the search gets lost. These features enable Xyntia to keep the advantages of Syntia (stability, output quality) while clearly improving over its weaknesses: especially Xyntia manages with 1s timeout to synthesize twice more expressions than Syntia with 10min timeout.

Other S-metaheuristics also perform significantly better than MCTS here, demonstrating that the problem itself is not well-suited for partial solution exploration and simulation-guided search.

6 COMPARE TO OTHER APPROACHES

We now extend the comparison to other state-of-the-art tools: (1) a greybox deobfuscator (QSynth [16]); (2) whitebox simplifiers (GCC, Z3 simplifier and our custom simplifier); (3) program synthesizers (CVC4 [6], winner of the SyGus’19 syntax-guided synthesis competition [2] and STOKE [30], an efficient superoptimizer). Unlike blackbox approaches, greybox and whitebox methods should be evaluated on the enhancement rate. Indeed, these methods can always succeed by returning the obfuscated expression without simplification. The enhancement rate measures how often synthesized expressions are smaller than the original (quality ≤ 1).

6.1 Experimental design

Xyntia and QSynth learn expressions over distinct grammars: Expr and MBA respectively. Moreover, QSynth is unfortunately not available, whether in a source or executable form. So we could neither adapt nor reproduce the experiments. In the end, we could only compare it over MBA, using the results reported by David et al. [16].

Benchmarks. We compare blackbox program synthesizers on B2 and grey/white box approaches on QSynth’s datasets – available for extended comparison. Thus, we consider the 3 datasets from David et al.’s [16] of obfuscated expressions using Tigress [11]: EA (base dataset, obfuscated with the EncodeArithmetic transformation), VR-EA (EA obfuscated with Virtualize and EncodeArithmetic protections), and EA-ED (EA obfuscated with EncodeArithmetic and EncodeData transformations).

6.2 Comparative evaluation

Greybox. We compare Xyntia to QSynth’s published results [16] on EA, VR-EA and EA-ED. Fig. 7a shows that while both tools reach comparable results (enhancement rate ≈ 350/500) for simple obfuscations (EA and VR-EA), Xyntia keeps the same results for
heavy obfuscations (EA-ED) while QSynth drops to 133/500. Actually, Xyntia is insensitive to syntactic complexity while QSynth is.

**Whitebox.** We compare Xyntia over the EA, VR-EA and EA-ED when time is limited. Results of STOKE-synth are also expected to Xyntia (Appendix A.3.1). Regardless of the obfuscation, they simplify \( \leq 1 \) and our custom simplifier. As expected, they are not efficient compared to Xyntia, GCC, Z3 simplifier (v4.8.7) as Xyntia (100 I/O samples with 5 constant vectors) as well as the datasets with 3 whitebox approaches: GCC, Z3 simplifier (v4.8.7) and our custom simplifier. As expected, they are not efficient compared to Xyntia (Appendix A.3.1). Regardless of the obfuscation, they simplify \( \leq 68 \) expressions where Xyntia simplifies 360 of them.

**Program synthesizers.** We now compare Xyntia to state-of-the-art program synthesizers, namely CVC4 [6] and STOKE [30]. CVC4 takes as input a grammar and a specification and returns, through enumerative search, a consistent expression. STOKE is a super-optimizer leveraging program synthesis (based on Metropolis Hastings) to infer optimized code snippets. It does not return an expression but optimized assembly code. STOKE addresses the optimization problem in two ways: (1) STOKE-synth starts from a pre-defined number of nops and mutates them, (2) STOKE-opti starts from the non-optimized code and mutates it to simplify it. While STOKE integrates its own sampling strategy and grammar, CVC4 does not – thus, we consider for CVC4 the same sampling strategy as Xyntia (100 I/O samples with 5 constant vectors) as well as the Expr and Mba grammars. More precisely, CVC4-Expr is used over B2 to compare to Xyntia (Xyntia\textsubscript{Opt}) and CVC4-Mba is evaluated on EA, VR-EA and EA-ED to compare against QSynth.

**Table 3: Program synthesizers on B2**

|                  | CVC4-Expr | STOKE-synth |
|------------------|-----------|-------------|
| Success Rate     | 36.8%     | 38.0%       |
| Equiv. Range     | 29.3 - 36.8% | 38.0%        |
| Mean Qual.       | 0.56      | 0.91        |

Table 3 shows that CVC4-Expr and STOKE-synth fail to synthesize more than 40% of B2 while Xyntia reaches 90.6% proven equivalence rate. Indeed enumerative search (CVC4) is less appropriate when time is limited. Results of STOKE-synth are also expected as its search space considers all assembly mnemonics. Moreover, Fig. 7a shows that blackbox and whitebox (STOKE-opti) synthesizers do not efficiently simplify obfuscated expressions. STOKE-opti finds only 1 / 500 expressions over EA-ED and does not handle jump instructions, inserted by the VM, failing to analyze VR-EA.

**6.3 Conclusion**

Xyntia rivals QSynth on light / mild protections and outperform it on heavy protections, while pure whitebox approaches are far behind, showing the benefits of being independent from syntactic complexity. Also, Xyntia outperforms state-of-the-art program synthesizers showing that it is better suited to perform deobfuscation. These good results show that seeing deobfuscation as an optimization problem is fruitful.

**7 DEOBFUSCATION WITH XYNTIA**

We now prove that Xyntia is insensitive to common protections (opaque predicates) as well as to recent anti-analysis protections (MBA, covert channels, path explosion) and we confirm that black-box methods can help reverse state-of-the-art virtualization [11, 35].

**7.1 Effectiveness against usual protections**

Xyntia is able to bypass many protections (Table 4).

**Mixed Boolean-Arithmetic** [38] hides the original semantics of an expression both to humans and SMT solvers. However, the encoded expression remains equivalent to the original one. As such, the semantic complexity stays unchanged, and Xyntia should not be impacted. Launching Xyntia on B2 obfuscated with Tigress [11] **Encode Arithmetic** transformation (size of expression: x800) confirms that it has no impact.

**Opaque predicates** [14] obfuscate control flow by creating artificial conditions in programs. The conditions are traditionally tautologies and dynamic runs of the code will follow a unique path. Thus, sampling is not affected and synthesis not impacted. We show it by launching Xyntia over B2 obfuscated with Tigress **Adaptive** transformation.

**Path-based obfuscation** [26, 36] takes advantage of the path explosion problem to thwart symbolic execution, massively adding additional feasible paths through dedicated encodings. We show that it has no effect, by protecting B2 with a custom encoding inspired by [26] (Appendix A.4.1 gives an example of our encoding).

**Covert channels** [32] hide information flow to static analyzers by rerouting data to invisible states (usually OS related) before retrieving it – for example taking advantage of timing difference between a slow thread and a fast thread to infer the result of some
We then used the scripts from [7] to sample each handler. Xyntia synthesizes 12/13 handlers in less than 7 s each. We can classify them in different categories: (1) arithmetic and Boolean (add, sub, mul, nor, and); (2) stack (store and load); (3) control flow (goto and return); (4) calling conversion (retrieve obfuscated function’s arguments). These results show that Xyntia can synthesize a wide variety of handlers. Interestingly, while these handlers contain many constant values (typically, offsets for context update), Xyntia can handle them as well. In particular, it infers the calling convention related handler, synthesizing constant values up to 28 (to access the 6th argument). Thus, even if Xyntia is inherently limited on constant values (see Section 5.6) it still handles them to a limited extent. Repeating the experiment by adding Encoded Data and Encode Arithmetic to Virtualize yields similar results. Xyntia synthesizes all 17 exposed handlers but one, confirming that Xyntia handles combinations of protections. Finally, note that Xyntia fails to synthesize handlers completely (not handling constant values). Still it infers arithmetic and Boolean handlers (without context updates).

We now use Xyntia to reverse code obfuscated with state-of-the-art virtualization. We obfuscate a program computing MBA operations with Tigress [11] and VMProtect [35] and our goal is to reverse the VM handlers. Using such synthetic program enables to expose a wide variety of handlers.

### Table 5: Xyntia and Syntia results over program obfuscated with Tigress [11] and VMProtect [35]

|                  | Tigress (simple) | Tigress (hard) | VMProtect |
|------------------|------------------|----------------|-----------|
| Binary size      | 40KB             | 251KB          | 615KB     |
| # handlers       | 13               | 17             | 114       |
| # instructions per handlers | 16               | 54             | 45        |
| Xyntia           | Completely retrieved 12/13 | 16/17 | 0/114 |
|                  | Partially retrieved 13/13 | 17/17 | 76/114 |
| Syntia           | Completely retrieved 0/13 | 0/17 | 0/114 |
|                  | Partially retrieved 13/13 | 17/17 | 76/114 |

**Tigress** [11] is a source-to-source obfuscator. Our obfuscated program contains 13 handlers. Since at assembly level each handler ends with an indirect jump to the next handler to execute, we were able to extract the positions of handlers using execution traces. We then used the scripts from [7] to sample each handler. Xyntia synthesizes 12/13 handlers in less than 7 s each. We can classify them in different categories: (1) arithmetic and Boolean (+, −, ×, ÷, ∧, ∨, ⊕); (2) stack (store and load); (3) control flow (goto and return); (4) calling conversion (retrieve obfuscated function’s arguments). These results show that Xyntia can synthesize a wide variety of handlers. Interestingly, while these handlers contain many constant values (typically, offsets for context update), Xyntia can handle them as well. In particular, it infers the calling convention related handler, synthesizing constant values up to 28 (to access the 6th argument). Thus, even if Xyntia is inherently limited on constant values (see Section 5.6) it still handles them to a limited extent. Repeating the experiment by adding Encoded Data and Encode Arithmetic to Virtualize yields similar results. Xyntia synthesizes all 17 exposed handlers but one, confirming that Xyntia handles combinations of protections. Finally, note that Xyntia fails to synthesize handlers completely (not handling constant values). Still it infers arithmetic and Boolean handlers (without context updates).

VMProtect [35] is an assembly to assembly obfuscator. We use the latest premium version (v3.5.0). As each VM handler ends with a ret or an indirect jump, we easily extracted each distinct handler from execution traces. Our traces expose 114 distinct handlers containing on average 43 instructions (Table 5). VMProtect’s VM is stack based. To infer the semantics of each handler, we again used Blazytko’s scripts [7] in “memory mode” (i.e., forbidding registers to be seen as inputs or outputs). Our experiments show that each arithmetic and Boolean handlers (add, mul, nor, and) are replicated 11 times to fake a large number of distinct handlers. Moreover, we are also able to extract the semantics of some stack related handlers.

### 7.2 Virtualization-based obfuscation

We now use Xyntia to reverse code obfuscated with state-of-the-art virtualization. We obfuscate a program computing MBA operations with Tigress [11] and VMProtect [35] and our goal is to reverse the VM handlers. Using such synthetic program enables to expose a wide variety of handlers.
Second, if the expression under analysis is too complex, the learner will fail to map inputs to their outputs.

In both cases, no information is retrieved. Hence, the key to impede blackbox obfuscation is to migrate from syntactic complexity to semantic complexity. We propose in Sections 8.2 and 8.3 two novel protections impeding the sampling and learning phases.

8.2 Semantically complex handlers

Blackbox approaches are sensitive to semantic complexity. As such, relying on a set of complex handlers is an effective strategy to thwart synthesis. These complex handlers can then be combined to recover standard operations. We propose a method to generate arbitrary complex handlers in terms of size and number of inputs.

**Complex semantic handlers.** Let $S$ be a set of expressions and $h, e_1, ..., e_{n-1}$ be $n$ expressions in $S$. Suppose that $(S, \star)$ is a group. Then $h$ can be encoded as $h = \prod_{i=0}^{n-1} h_i$, where for all $i$, with $0 \leq i \leq n$,

$$h_i = \begin{cases} h - e_1 & \text{if } i = 0 \\ e_i - e_{i+1} & \text{if } 1 \leq i < n - 1 \\ e_{n-1} - e_{n-2} & \text{if } i = n - 1 \end{cases}$$

Each $h_i$ is a new handler that can be combined with others to express common operations – see Table 6 for an example. Note that the choice of $(e_1, ..., e_n)$ is arbitrary. One can choose very complex expressions with as many arguments as wanted.

Table 6: Examples of encoding

| $h_0$ | $(x + y) - (-((a - x^2) - (xy)))$ |
|-------|----------------------------------|
| $h_1$ | $(a - x^2) - xy + ((y - (a \land x)) \times (y \oplus x))$ |
| $h_2$ | $(y - (a \land x)) \times (y \oplus x)$ |
| $h$   | $x + y$                           |

**Experimental design.** To evaluate Syntia and Xyntia against our new encoding, we created 3 datasets – BP1, BP2 and BP3, listed by increasing order of complexity. Each dataset contains 15 handlers which can be combined to encode the $+, -, \land, \lor$ operators. Within dataset, all handlers have the same number of inputs. Table 7 reports details on each dataset – more details are available in Appendix A.5. The mean overhead column is an estimation of the complexity added to the code by averaging the number of operators needed to encode a single basic operator ($+, -, \land, \lor$). Overheads in BP1 (21x), BP2 (39x) and even BP3 (258x) are reasonable compared to some syntactical obfuscations: encoding $x + y$ with MBA three times in Tigress yields a 800x overhead.

**Evaluation.** Results (Fig. 8) show that while Xyntia (with 1h.expr.) manages well low complexity handlers (BP1: 13/15), yet performance degrades quickly as complexity increases (BP2: 3/15, BP3: 1/5). Syntia, CVC4 and STOKE-synth find none with 1 h/expr., even on BP1 (Appendix A.5).

Table 7: Protected datasets

| #exprs | min size | max size | mean size | #inputs | mean overhead |
|--------|----------|----------|-----------|---------|---------------|
| BP1    | 15       | 4        | 11        | 6.87    | 3             | x21          |
| BP2    | 15       | 8        | 21        | 12.87   | 6             | x39          |
| BP3    | 15       | 58       | 142       | 86.07   | 6             | x258         |

**Conclusion.** Semantically complex handlers are efficient against blackbox obfuscation. While high complexity handlers come with a cost similar to strong MBA encodings, medium complexity handlers offer a strong protection at a reasonable cost.

**Discussion.** Our protection can be bypassed if the attacker focuses on the good combinations of handlers, rather than on the handlers themselves. To prevent it, complex handlers can be duplicated (as in VMProtect, see Section 7.2) to make patterns recognition more challenging.

![Figure 8: Xyntia (Xyntia0Fp) on BP1, 2, 3 – varying timeouts](image)

8.3 Merged handlers

We now propose another protection, based on conditional expressions and the merging of existing handlers. While block merging is known for a long time against human reversers, we show that it is extremely efficient against blackbox attacks. Note that while we write our merged handlers with explicit if-then-else operators (ITE) for simplicity, these conditions are not necessarily implemented with conditional branching (cf. Fig. 9 for an example of branchless encoding). Hence, we consider that the attacker sees merged handlers as a unique code fragment.

**Datasets.** We introduce 5 datasets (see Appendix A.5.2) composed of 20 expressions. Expressions in dataset 1 are built with 1 if-then-else (ITE) exposing 2 basic handlers (among $+, -, \land, \lor, \oplus$); expressions in dataset 2 are built with 2 nested ITEs exposing 3 basic handlers, etc. Conditions are equality checks against consecutive constant values (0, 1, 2, etc.). For example, dataset 2 contains the expression:

$$ITE(z = 0, x + y, ITE(z = 1, x - y, x \times y))$$

(2)

**Scenarios.** Adding conditionals brings extra challenges (1) the grammar must be expressive enough to handle conditions; (2) the sampling phase must be efficient enough to cover all possible behaviors. Thus, we consider different scenarios:

- **Utopian** The synthesizer learns expressions over the MBA set of operators, extended with an ITE ($\star = 0, \star, \star$) operator (MBA+ITE operator set). Moreover, the sampling is done so that all branches are traversed the same number of time. This situation, favoring the attacker, will show that merged handlers are always efficient.

- **MBA + ITE** This situation is more realistic: the attacker does not know at first glance how to sample. However, its grammar fits perfectly the expressions to reverse.

| Available at: Will be made available |
\[ \text{Mba + Shifts} \] Here Xyntia does not sample inputs uniformly over the different behaviors, does not consider ITE operators, but allows shifts to represent branch-less conditions.

\[ \text{Default} \] This is the default version of the synthesizer.

In all these scenarios, appropriate constant values are added to the grammar. For example, to synthesize Eq. (2), \( \theta \) and 1 are added.

```c
int32_t h(int32_t a, int32_t b, int32_t c) {
  // if (c == cst) then h1(a,b,c) else h2(a,b,c);
  int32_t res = c - cst;
  int32_t s = res >> 31;
  res = (-((res * s) -s) >> 31) & 1;
  return h1(a, b, c)*(1 - res) + res*h2(a, b, c);
}
```

**Figure 9: Example of a branch-less condition**

**Evaluation** Fig. 10 presents Xyntia’s results on the 5 datasets. As expected, the Utopian scenario is where Xyntia does best, still it cannot cope with more than 3 nested ITEs. For realistic scenarios, Xyntia suffers even more. Results for Syntia, CVC4 and STOKESynth (see Appendix A.5.2) confirm this result (no solution found for \( \geq 2 \) nested ITEs). Note that overhead here is minimal, as the merging only add a few conditional jumps.

**Conclusion**. Merged handlers are extremely powerful against blackbox synthesis. Even in the ideal sampling scenario, blackbox methods cannot retrieve the semantics of expressions with more than 3 nested conditionals – while runtime overhead is minimal.

**Discussion**. Symbolic methods, like symbolic execution, are unhindered by this protection, for they track the succession of handlers and know which sub parts of merged handlers are executed. They can then reconstruct the real semantics of the code. To handle this, our anti-AI protection can be combined with (lightweight) anti-symbolic protections (e.g. \([26, 36]\)).

9 RELATED WORK

**Blackbox deobfuscation.** Blazytko et al.’s work \([7]\) has already been thoroughly discussed. We complete their experimental evaluation, generalize and improve their approach: Xyntia with 1s/expr. finds twice more expressions than Syntia with 600s/expr.

**White- and greybox deobfuscation.** Several recent works leverage whitebox symbolic methods for deobfuscation (“symbolic deobfuscation”) \([5, 10, 22, 29, 31, 37]\). Unfortunately, they are sensitive to code complexity as discussed in Section 7, and efficient countermeasures are now available \([12, 26, 27, 38]\) – while Xyntia is immune to them (Section 7.1). David et al. \([16]\) recently proposed QSynth, a greybox deobfuscation method combining I/O relationship caching (blackbox) and incremental reasoning along the target expression (whitebox). Yet, QSynth is sensitive to massive syntactic obfuscations where Xyntia is not (cf. Section 6). Furthermore, QSynth works on a simple grammar. It is unclear whether its caching technique would scale to larger grammars like those of Xyntia and Syntia.

**Program synthesis.** Program synthesis aims at finding a function from a specification which can be given either formally, in natural language or as I/O relations – the case we are interested in here. There exist three main families of program synthesis methods \([20]\): enumerative, constraint solving and stochastic. Enumerative search does enumerate all programs starting from the simpler one, pruning snippets incoherent with the specification and returning the first code meeting the specification. We compare, in this paper, to one of such method – CVC4 \([6]\), winner of the SyGuS ’19 syntax-guided synthesis competition \([2]\) – and showed that our approach is more appropriate to deobfuscation. Constraint solving methods \([21]\) on the other hand encode the skeleton of the target program as a first order satisfiability problem and use an off-the-shelf SMT solver to infer an implementation meeting specification. However, it is less efficient than enumerative and stochastic methods \([1]\). Finally, stochastic methods \([30]\) traverse the search space randomly in the hope of finding a program consistent with a specification. Contrary to them, we aim at solving the deobfuscation problem in a fully blackbox way (not relying on the obfuscated code, nor on an estimation of the result size).

10 CONCLUSION

AI-based blackbox deobfuscation is a promising recent research area. The field has been barely explored yet and the pros and cons of such methods are still unclear. This article deepens the state of AI-based blackbox deobfuscation in three different directions. First, we define a novel generic framework for AI-based blackbox deobfuscation, encompassing prior works such as Syntia, we identify that the search space underlying code deobfuscation is too unstable for simulation-based methods, and advocate the use of S-metaheuristics. Second we take advantage of our framework to carefully design Xyntia, a new AI-based blackbox deobfuscator. Xyntia significantly outperforms Syntia in terms of success rate, while keeping its good properties – especially, Xyntia is completely immune to the most recent anti-analysis code obfuscation methods. Xyntia also proves to be more efficient than greybox and whitebox deobfuscators or standard program synthesis methods. Finally, we propose the two first protections against AI-based blackbox deobfuscation, completely preventing Xyntia and Syntia’s attacks for reasonable cost. We hope that these results will help better understand AI-based deobfuscation, and lead to further progress in the field.
A APPENDIX

We now introduce complementary results to describe details that we did not fully explain for the sake of space. We follow the same organisation as the main article:

Appendix A.1 details the evaluation of Syntia (from Section 4). It presents used datasets and obtained Syntia results;

Appendix A.2 details the evaluation of Xyntia (see Section 5) and the study leading to the optimal Xyntia;

Appendix A.3 describes the comparison of Xyntia to white-box, pattern based simplifiers from Section 6.

Appendix A.4 details the obfuscations used to evaluate Xyntia against state-of-the-art protections in Section 7;

Appendix A.5 describes datasets used in Section 8 and details evaluation of Syntia, CVC4 and STOKE over proposed protections.

A.1 Understand AI-based deobfuscation: More Details

Section 4 presents an in-depth evaluation of Syntia. We show now complementary data to detail: (1) the distribution of expressions in our custom benchmark suite B2; (2) the results of Syntia over 15 runs; (3) the results of Syntia in terms of quality and correctness and how it reacts to the number of inputs and expression types; (4) the study of Syntia’s parameters to find an optimal configuration.

Table 8: Description of B2

| Type   | # Inputs |
|--------|----------|
| Bool.  | 150      |
| Arith. | 600      |
| MBA    | 180      |
| 2      | 90       |
| 3      | 90       |

A.1.1 Experimental design. In order to perform a fine grained evaluation of Syntia, we use 2 benchmark suites: B1 and B2. B1 has been introduced by Blazzytko et al. [7] to evaluate Syntia, and contains 500 expressions. However, it presents important limitations as discussed in Section 4.2. Thus, we introduce a custom benchmark B2 which contains 1110 expressions. It is better distributed according to the type of the expressions – Boolean, Arithmetic and Mixed Boolean-Arithmetic – and number of inputs used – between 2 and 6. Moreover, B2 is more challenging than B1, considering more complex expressions. Table 8 presents the number of expressions per type of expressions and number of inputs.

A.1.2 Evaluation of Syntia. In Section 4.2 we evaluate Syntia to estimate its stability across executions, its robustness, speed, quality and correctness. We present now complete experiments results and discuss them.

RQ1. Table 9 presents results of Syntia over 15 runs and Table 10 presents statistics on it. We observe that Syntia is indeed very stable across executions.

RQ2. As presented in Table 10 Syntia is not able to synthesize B2 efficiently, only synthesizing 34.5% of it. Moreover, as presented in Table 26, Syntia cannot handle expressions using more than 3 inputs. Indeed, its success rate falls to 10.0%, 2.2% and 1.1% for respectively 4, 5 and 6 inputs. Syntia is also impacted by the type of the target expression. Handling boolean expressions seems simpler for Syntia. On the contrary, it struggles to synthesize MBA expressions. Still we observe that Syntia returns really good quality results (≈ 0.60) and almost never returns non equivalent expressions.

RQ3. Syntia defaults to synthesizing expressions over the Full operators’ set. To evaluate its sensitivity to the size of the operators’ set, we launch it over Full,Expr and MBA. Table 11 shows that restricting the search space benefits to Syntia. However, even in the best scenario (MBA) its results are deceiving. Indeed, it synthesizes only ≈ 42% of B2.

Table 9: Success rate of Syntia across 15 runs (timeout=60s)

| Test execution no. | B1 | B2 |
|--------------------|----|----|
| 1                  | 367 (73.4%) | 349 (31.4%) |
| 2                  | 362 (72.4%) | 376 (33.9%) |
| 3                  | 376 (75.2%) | 371 (33.4%) |
| 4                  | 365 (73.0%) | 367 (33.1%) |
| 5                  | 369 (73.8%) | 379 (34.1%) |
| 6                  | 365 (73.0%) | 383 (34.5%) |
| 7                  | 375 (75.0%) | 366 (33.0%) |
| 8                  | 370 (74.0%) | 371 (33.4%) |
| 9                  | 366 (73.2%) | 358 (32.3%) |
| 10                 | 372 (74.4%) | 367 (33.1%) |
| 11                 | 367 (73.4%) | 364 (32.8%) |
| 12                 | 364 (72.8%) | 372 (33.5%) |
| 13                 | 371 (74.2%) | 378 (34.1%) |
| 14                 | 368 (73.6%) | 350 (31.5%) |
| 15                 | 370 (74.0%) | 354 (31.9%) |

Table 10: 15 runs of Syntia over B1 and B2 (timeout = 60 s)

| Data-set | Min. | Max. | Mean | σ |
|----------|------|------|------|---|
| Syntia   | 362 (72.4%) | 376 (75.2%) | 368.5 (73.7%) | 3.83 (0.76%) |
| B2       | 349 (31.4%) | 383 (34.5%) | 367.0 (33.1%) | 10.11 (0.91%) |

A.1.3 Optimal Syntia. To ensure conclusions given in Section 4.4 apply to MCTS and not only to Syntia, we studied Syntia extensively, searching for better set-ups. We study Syntia according to following parameters: simulation depth, SA-UCT value, number of I/O samples and choice of the distance.

Table 12: Syntia depending on max playout depth (MBA, B2, timeout = 60 s).

| Max play. depth | 0 | 3 | 5 |
|-----------------|---|---|---|
| Succ. Rate      | 42.6 % | 31.8 % | 28.6 % |
| Equiv. Range    | 42.3 - 42.6 % | 31.4 - 31.8 % | 28.1 - 28.6 % |
| Mean Qual.      | 0.66 | 1.03 | 1.06 |
Simulation depth. As presented in Section 4.4, MCTS simulates each generated nodes. To do so, it applies rules of the grammar randomly to the non terminal expression until it becomes terminal. An important parameter is thus the maximum simulation depth i.e. the number of rules not leading to terminal nodes (like $U \rightarrow U+U$). By default, Syntia considers a maximum simulation depth of 0, which mean that all non terminal symbols are directly replaced by variables or constant values. Table 12 shows that increasing this parameter is not beneficial.

Number of I/O samples. By defaults, Syntia considers 50 samples. Table 13 presents results for different number of samples. We observe little improvement when the number of samples decreases. Still, it stays in the same range of results.

Table 13: Syntia for different number of samples (B2, M/b.sc/a.sc, timeout=60s).

| # samples | 10 | 20 | 50 | 100 |
|-----------|----|----|----|-----|
| Succ. Rate| 45.6% | 44.9% | 42.6% | 43.2% |
| Equiv. Range| 45.1 - 45.4% | 44.7 - 44.9% | 42.3% - 42.6% | 42.9 - 43.2% |
| Mean Qual. | 0.69 | 0.71 | 0.66 | 0.69 |

Objective function. By default, Syntia evaluates if an expression is close to the target one by computing the mean between different distances. To complete our evaluation of Syntia we launched it with Xyntia’s Log-arithmetic distance. We observe that as Xyntia the log-arithmetic seems more appropriate to guide the search. Still, Syntia’s success rate stays below 50%.

Table 14: Syntia depending on the objective function (B2, M/b.sc/a.sc, timeout=60s).

| Objective function | Syntia-dist | Log-arith |
|--------------------|-------------|-----------|
| Succ. Rate | 42.6% | 47.9% |
| Equiv. Range | 42.3% - 42.6% | 47.4 - 47.9% |
| Mean Qual. | 0.66 | 0.70 |

Simulated annealing UCT (SA-UCT). From a high level, MCTS can be divided in 2 behaviors: exploitation (where it focuses on promising nodes) and exploration (where it checks rarely visited or at first glance non interesting nodes). The SA-UCT constant is a parameter to configure the balance between these behaviors. The smaller is the constant the more exploitative MCTS is. On the contrary, the bigger it is, more explorative is MCTS. By default Syntia sets the SA-UCT constant to 1.5. Table 15 presents results of Syntia for smaller and bigger values. For smaller values, Syntia is less efficient. This is coherent with claims from Section 4.4. Indeed, as the search space is highly unstable, simulations are misleading. Thus, focusing too much on exploitation is unsuitable. However, it also appears that, bigger values can be beneficial. This is also coherent with Section 4.4 as it shows that the most important behavior is exploration. Still, even with SA-UCT values > 1.5 success rate stays low (< 50%).

Optimal Syntia. Our extensive study highlights a new optimal configuration of Syntia (M/b.sc set of operators, simulation depth=0, #samples=10, objective function=log-arithmetic, SA-UCT=2). However, even with this configuration, Syntia success rate stays around 50% (Table 16). While slightly better, such results are still disappointing.

Table 15: Syntia depending on SA-UCT value (M/b.sc, B2, timeout = 60 s).

| SA-UCT | Succ. Rate | Equiv. Range | Mean Qual. |
|--------|------------|--------------|------------|
| 1      | 48.0% | 47.7 - 48.0% | 0.71 |
| 2      | 48.2% | 48.1 - 48.2% | 0.72 |
| 1.5    | 42.6% | 42.3% - 42.6% | 0.66 |
| 0.5    | 34.6% | 42.9 - 43.2% | 0.62 |
| 0.1    | 19.1% | 47.4 - 47.9% | 0.44 |

Table 16: Optimal Syntia (B2, timeout = 60 s).

| Test execution no. | B1  | B2  |
|--------------------|-----|-----|
| 1                  | 500 (100%) | 1051 (94.7%) |
| 2                  | 500 (100%) | 1051 (94.7%) |
| 3                  | 500 (100%) | 1060 (95.5%) |
| 4                  | 500 (100%) | 1054 (95.0%) |
| 5                  | 500 (100%) | 1060 (95.5%) |
| 6                  | 500 (100%) | 1059 (95.4%) |
| 7                  | 500 (100%) | 1051 (94.7%) |
| 8                  | 500 (100%) | 1059 (95.4%) |
| 9                  | 500 (100%) | 1055 (95.0%) |
| 10                 | 500 (100%) | 1053 (94.7%) |
| 11                 | 500 (100%) | 1059 (95.4%) |
| 12                 | 500 (100%) | 1052 (94.8%) |
| 13                 | 500 (100%) | 1061 (95.6%) |
| 14                 | 500 (100%) | 1054 (95.0%) |
| 15                 | 500 (100%) | 1053 (94.9%) |

A.2 Improve AI-based deobfuscation: More details

Section 5 presents our new AI-based blackbox deobfuscator dubbed Xyntia. We show now complementary data and results to detail: (1) the results of Xyntia over 15 runs; (2) the results of Xyntia in terms of quality, correctness, capacity to handle high number of inputs and different expression types; (3) the results of Xyntia over FULL, EXPR, MBA; (4) the study leading to optimal Xyntia; (5) the capacity of Xyntia to integrate a high number of constant values in its grammar.

A.2.1 Evaluation of Xyntia. To evaluate Xyntia and compare it against Syntia we replicate for Xyntia the experimental procedure followed in Section 4. We present now complete experiments results and discuss them.

RQ4. To assess the usability of Xyntia we need to know if it is stable across executions. Indeed, Xyntia, as Syntia, is stochastic and results may vary from one run to another. Table 17 shows results of Xyntia over 15 runs on B1 and B2 – statistics are given in Table 18. No significant variation is observed, meaning that Xyntia is stable across executions.

Table 17: Success rate of Xyntia (XyntiaOpt) across 15 runs (timeout = 60 s).

| Test execution no. | B1  | B2  |
|--------------------|-----|-----|
| 1                  | 1051 (94.7%) | 1051 (94.7%) |
| 2                  | 1051 (94.7%) | 1060 (95.5%) |
| 3                  | 1054 (95.0%) | 1060 (95.5%) |
| 4                  | 1059 (95.4%) | 1059 (95.4%) |
| 5                  | 1055 (95.0%) | 1059 (95.0%) |
| 6                  | 1053 (94.7%) | 1055 (95.0%) |
| 7                  | 1054 (95.0%) | 1059 (95.4%) |
| 8                  | 1059 (95.4%) | 1059 (95.4%) |
| 9                  | 1053 (94.7%) | 1055 (95.0%) |
| 10                 | 1054 (95.0%) | 1059 (95.4%) |
| 11                 | 1052 (94.8%) | 1061 (95.6%) |
| 12                 | 1054 (95.0%) | 1053 (94.7%) |
| 13                 | 1053 (94.7%) | 1059 (95.4%) |
| 14                 | 1053 (94.7%) | 1055 (95.0%) |
| 15                 | 1053 (94.9%) | 1053 (94.9%) |

RQ5. Unlike Syntia, Xyntia is efficient on B2. Moreover, as presented in Table 19, it is able to synthesize expressions using up to 5 inputs with a success rate ≥ 80%. Even for 6 inputs it still
Table 18: Xyntia (Xyntia_{OPT}): 15 runs on B1/B2 (timeout=60s)

| Data-set | Min.   | Max.   | Mean   | σ      |
|----------|--------|--------|--------|--------|
| Xyntia   |        |        |        |        |
| B1       | 500(100%) | 500(100%) | 500(100%) | 0(0.00%) |
| B2       | 1051(94.7%) | 1061(95.6%) | 1055.5(95.1%) | 3.63(0.33%) |

reaches a success rate > 70%. Furthermore, it enables to synthesize efficiently different types of expressions. While it seems harder to synthesize MBA expressions, even for Xyntia, it still synthesizes > 85% of them. In addition, we observe that Xyntia returns simple and almost always correct results. Still, results given in Table 19 seems to show that Xyntia returns better quality results and less non-equivalent expressions than Xyntia. However, these conclusions are biased by the fact that Xyntia has a lower success rate than Xyntia and finds only very simple expressions. Thus, we present results on expressions that had been successfully synthesized by both Syntia and Xyntia. Table 20 demonstrates that under this condition, the quality of both tools are comparable. Still, Xyntia reaches such results thanks to our post-process simplifier. Thus, Xyntia effectively synthesizes simpler expressions, but the gap can be bridged by adding a simple simplifier to Xyntia. On the other hand, we see that Syntia returns between 6 and 9 non-equivalent expressions while Xyntia returns between 1 and 4. Thus Xyntia seems more reliable.

RQ6. Xyntia defaults to synthesizing expressions over Expr while Syntia infers expressions over Full. To evaluate the sensitivity of Xyntia to search space and show that previous results was not due to search space inconsistency, we run Xyntia over Full, Expr and MBA. Table 21 indicates that Xyntia reaches high equivalence rates for all operators’ sets – recall Syntia results stayed low. Still, Xyntia seems more sensitive to the size of the set of operators than Syntia. Its proven equivalence rate decreases from 90% (Expr) to 71% (Full) while Syntia decreases only from 38.7% (Expr) to 33.7% (Full). On the other hand, restricting the search space to MBA benefits to both Syntia and Xyntia.

A.2.2 Optimal Xyntia. The systematic evaluation of Xyntia depending on some design choices is resumed in Section 5.4. We complete here our analysis and give more details about the measured results. We focus on the following aspects: (1) the choice of the S-metahuristic; (2) the choice of the sampling strategy; (3) the choice of the distance as objective function; (4) the effect of our custom simplifier.

Choice of the S-metahuristic. We compare 5 S-metaheristics, namely Hill Climbing, Random Walk, Simulated Annealing, Metropolis Hasting and Iterated Local Search, to find out the better suited to deobfuscation. Table 22 shows that ILS has a higher equivalence rate than other search heuristics. Moreover, we observe that all S-metaheristics obtain similar or better results than Syntia. The low equivalence rate of Hill Climbing compared to other S-metaheristics can be explained by the fact that it has no way to evade local optimums. Even in this conditions, we observe that its results are not that far from Syntia (which reaches an equivalence rate of ≈ 38% on Expr). It confirms that estimating non terminal expression’s pertinence through simulations as MCTS does is not suitable for deobfuscation (see Section 4.4). It is far more relevant to manipulate terminal expressions only as S-metaheristics do.

Effect of the sampling strategy. Table 23 presents Xyntia’s results for different number of randomly chosen I/O samples. Intuitively, the higher the number of samples is considered, the more precise is the synthesis specification. Consequently, one may think that increasing the number of samples would negatively impact the success rate and positively impact the equivalence rate. The experiments shows that while it improves the equivalence rate (from 74.95% to 87.39% for respectively 10 and 100 I/O samples on Expr), it does not weaken the success rate. This result can be explained by the fact that more inputs are used by the objective function to more precisely guide the synthesis. Still, the degree to which the results are impacted depends on the set of operators. For MBA and Expr, the equivalence range seems to stagnate when adding more than 50 samples while Full still improves with 100 samples.

In order to improve Xyntia’s results over the Full sets of operators we propose to add constant vectors (0, 1, -1, min, max) to enforce important behaviors such as division by zero and overflows. Table 24 presents results of Xyntia in two configurations: (1) 100 randomly generated samples and (2) 95 randomly generated samples plus 5 constant vectors. We see that adding such constant vectors slightly improves Xyntia’s equivalence rate over the Full and Expr sets of operators.

Choice of the distance. The default design of Xyntia (Section 5) leverages the Log-arithmetic distance as objective function. We present in Table 25 an evaluation of Xyntia with the following alternative distances:

- Arithmetic $d_{\text{ar}}(\bar{o}) = \sum |o_i - o_i^*|$
- Hamming $d_{\text{h}}(\bar{o}) = \sum_{i=0}^{31} o_{i,j} \oplus o_{i,j}^*$
- Xor $d_{\text{x}}(\bar{o}) = \sum_{i=0}^{31} o_i \oplus o_i^*$
- Log-Arithmetic $d_{\text{lar}}(\bar{o}) = \sum_{i=0}^{31} \log_2(1 + |o_i - o_i^*|)$

where $\bar{o}^*$ is the vector of sampled outputs and $\bar{o}$ is the actual outputs of the synthesized expression.

It appears that the Log-arithmetic distance guides synthesis the best. Over Expr, Xyntia reaches a proven equivalence rate between 84.50% with the Hamming distance, and 90.6% with the Log-arithmetic one. While, intuitively, the Xor and Hamming distances should guide the search better for Boolean expressions, Table 26 demonstrates that this is not the case: the Log-arithmetic distance as objective function. We leverage the Log-arithmetic distance as objective function. We present in Table 25 an evaluation of Xyntia with the following alternative distances:

Effect of the simplifier. Xyntia integrates a simple and efficient simplification engine to post-process the expressions found. The simplification rules, which are partially listed in Table 28, are iteratively applied on the expression until a fixpoint is reached. Table 27 presents the quality of synthesized expressions with and without the simplification engine. We observe that the simplifier significantly improves the quality of the expressions and enables us to reach really good quality results (%1) for Expr and MBA. However, for Full, the quality stays around 1.3. As such, some more engineering might be needed to get better results for Full. Nevertheless, our simplifier efficiently rewrite expressions while adding no significant latency. Indeed, the average time spent with this post-processing step is around 2.6ms.
Table 19: Syntia & Xyntia (Xyntia\textsubscript{OPT}): results according to expression type and number of inputs (B2, timeout = 60 s)

| Type | Property | Bool. | Arith. | MBA | 2 | 3 | 4 | 5 | 6 | All |
|------|----------|-------|--------|-----|---|---|---|---|---|-----|
|      | Succ. Rate | 53.8% | 28.6% | 21.1% | 77.3% | 41.0% | 10.0% | 2.2% | 1.1% | 34.5% |
|      | Equiv. Range | 53.0% | 27.8% - 28.1% | 20.3% - 20.8% | 74.0% - 75.33% | 40.3% - 40.5% | 10.0% | 2.2% | 1.1% | 33.7% - 34.0% |
|      | Mean Qual. | 0.53 | 0.61 | 0.71 | 0.57 | 0.60 | 0.67 | 0.12 | 0 | 0.59 |
|      | Succ. Rate | 98.4% | 96.5% | 91.6% | 98.7% | 98.8% | 98.9% | 82.2% | 74.4% | 95.5% |
|      | Equiv. Range | 97.8% | 88.9% - 94.9% | 85.1% - 90.0% | 93.3% - 97.3% | 93.2% - 97.7% | 94.4% - 97.2% | 80.0% - 81.1% | 72.2% - 73.3% | 90.6% - 94.2% |
|      | Mean Qual. | 0.73 | 1.0 | 1.05 | 0.68 | 0.90 | 1.1 | 0.94 | 1.05 | 0.92 |

Table 20: Results for expressions that both Syntia and Xyntia (Xyntia\textsubscript{OPT}) successfully synthesized (B2, timeout = 60 s).

| | Syntia | Xyntia |
|---|---|---|
| #Succ. | 383 | 383 |
| #Equiv. | 374 - 377 | 379 - 382 |
| Mean Qual. | 0.58 | 0.62 |

Table 21: Xyntia (Xyntia\textsubscript{OPT}): results on F/u.sc/l.sc/l.sc, E/x.sc/p.sc/r.sc and M/b.sc/a.sc (B2, timeout = 60 s).

| | Arith | MBA |
|---|---|---|
| Succ. Rate | 85.3% | 86.3% |
| Equiv. Range | 71.2% - 76.1% | 90.6% - 94.2% |
| Mean Qual. | 1.04 | 0.97 |

Table 22: Synthesis Equivalence Rate for different S-metaheuristics (B2, Xyntia\textsubscript{OPT}, timeout = 60 s).

| S-metaheuristic | Equiv. Range |
|---|---|
| Random Walk | 62.3% - 63.4% |
| Hill Climbing | 31.9% - 33.1% |
| Iterated Local Search | 90.6% - 94.2% |
| Simulated Annealing | 64.8% - 65.8% |
| Metropolis-Hastings | 57.7% - 58.5% |

Table 23: Results of Xyntia for different number of samples (B2, Xyntia\textsubscript{OPT}, timeout = 60 s).

| # samples | FULL | EXPR | MBA |
|---|---|---|---|
| Succ. Rate | 86.58% | 94.50% | 95.59% |
| Equiv. Range | 69.55% - 76.22% | 87.57% - 93.51% | 89.37% - 95.59% |
| Mean Qual. | 1.14 | 0.98 | 1.01 |

Table 24: Xyntia with and without constant values (B2, Xyntia\textsubscript{OPT}, timeout = 60 s).

| | FULL | EXPR | MBA |
|---|---|---|---|
| Succ. Rate | 86.67% | 95.32% | 96.58% |
| Equiv. Range | 69.10% - 75.50% | 87.39% - 93.51% | 91.26% - 96.58% |
| Mean Qual. | 1.05 | 0.94 | 0.95 |

Table 25: Xyntia’s results for different distances (B2, Xyntia\textsubscript{OPT}, timeout = 60 s).

| Dist. | FULL | EXPR | MBA |
|---|---|---|---|
| Succ. Rate | 86.58% | 94.50% | 95.59% |
| Equiv. Range | 69.55% - 76.22% | 87.57% - 93.51% | 89.37% - 95.59% |
| Mean Qual. | 1.14 | 0.98 | 1.01 |

we propose to discuss here if AI-based blackbox methods can efficiently synthesize expressions manipulating constant values. Indeed, Xyntia and Syntia only integrate the constant 1 in their grammar. Thus, if they try to synthesize an expression containing constant values (≠ 1) they will need to create them. However, this is unlikely, especially if the constant is far from 1. One solution is to add all $2^{32}$ constant values in the grammar. In order to verify if this approach is conceivable, we add ranges of constant values ([1; $u_1D441$]) for $u_1D441$ ∈ {1, 10, 50, 100, 200} in Xyntia’s grammar. The results for each configuration are presented in Fig. 11. They show that increasing the number of constant values dramatically impacts Xyntia’s performance. We conclude that adding all possible constant values is not beneficial. Another solution is to add well chosen constant values (-1, $u_1D45A/u_1D456/u_1D45B$ /u1D460, $u_1D45A/u_1D44E/u_1D465$ /u1D460) but we decided not to explore this approach in this paper. Still, in Section 7.2, we observe that such restriction is limited as Xyntia is able to synthesize interesting constant values. Note that Syntia cannot do it.

A.2.3 Limitations. Section 5.6 discusses inherent limitations of blackbox methods. While some are extensively studied in Section 8,
Table 26: Xyntia’s results for different distances over Boolean and arithmetic type of expressions (B2, XyntiaOpt, timeout = 60 s).

| Dist. | Boolean | Arith. |
|-------|---------|--------|
| Arith | Succ. Rate | 96.76% | 96.49% |
|       | Equiv. Range | 95.68% - 95.68% | 87.30 - 95.68% |
|       | Mean Qual. | 0.75 | 1.05 |
| Hamm. | Succ. Rate | 97.84% | 90.81% |
|       | Equiv. Range | 95.41 - 95.68% | 81.08 - 89.19% |
|       | Mean Qual. | 0.79 | 0.97 |
| Xor   | Succ. Rate | 98.38% | 96.48% |
|       | Equiv. Range | 97.84% - 95.14% | 82.16 - 87.03% |
|       | Mean Qual. | 0.76 | 0.98 |

Table 27: Xyntia quality with and without simplifier (B2, XyntiaOpt, timeout = 60 s).

|          | FULL | EXPR | MBA |
|----------|------|------|-----|
| Mean Qual. No Simpl. | 1.77 | 1.33 | 1.38 |
| Mean Qual. Simpl. | 1.19 | 0.93 | 0.97 |
| Mean Simpl. Time (s) | 0.0027 | 0.0026 | 0.0026 |

Figure 11: Effect of the number of constant values in Xyntia’s grammar on equivalence rate (B2, XyntiaOpt, timeout=60s)

A.3 Compare to other approaches: More details

We present in Section 6 a comparative study of Xyntia against grey-box deobfuscators, whitebox simplifiers and state-of-the-art program synthesizers. We give here more details on how Xyntia compares to whitebox simplifiers.

A.3.1 Comparison to whitebox simplifiers. We compare Xyntia over the EA, VR-EA and EA-ED datasets with 3 whitebox approaches: GCC, Z3 simplifier (v4.8.7) and our custom simplifier. We use GCC v8.3.0 with optimization level 3 to compile obfuscated expressions. We do not report the mean simplification time of GCC because our measurements consider the whole compilation process which would not be fair compared to other methods. We extract expressions’ semantics through decompilation for EA and EA-ED datasets (using ghidra [25]) and leverage symbolic execution using Binsec [15] for VR-EA dataset where it is not possible to use decompilation. Because, our custom simplification engine does not integrate concatenation simplification, it did not simplify any expressions over VR-EA. Table 29 shows that GCC, Z3 simplify and our custom simplifier hardly clear expressions compared to Xyntia. However, synthesis is on average slower that syntax based simplifiers.

Table 28: Xyntia’s simplification rules (partial)

| Constant | $f(\text{const}_1, \ldots, \text{const}_N)$ | → | result |
|----------|--------------------------------------|---|--------|
| $E_1 + 0$ | $E_1$ |
| $E_1 - 0$ | $E_1$ |
| $E_1 \land \lnot E_2$ | $E_1 + E_2$ |
| $E_1 \land \lnot E_2$ | $E_1$ |
| $E_1 \lor 0$ | $E_1$ |
| $E_1 \lor \lnot E_1$ | $E_1$ |
| $E_1 \lor \lnot E_1$ | $E_1$ |
| $E_1 \land 0$ | $E_1$ |

Table 29: Results of whitebox simplifiers on the EA dataset

|          | GCC -03 | Simplifier | Z3 | Xyntia |
|----------|---------|------------|----|--------|
| EA       | Enhancement rate | 68 / 500 | 36 / 500 | 22 / 500 | 360 / 500 |
|          | Mean time (s) | 0.0005 | 0.0002 | 2.45 |
| VR-EA    | Enhancement rate | 22 / 500 | 0 / 500 | 31 / 500 | 360 / 500 |
|          | Mean time (s) | 0.0010 | 0.00042 | 2.45 |
| EA-ED    | Enhancement rate | 14 / 500 | 15 / 500 | 17 / 500 | 360 / 500 |
|          | Mean time (s) | 0.0055 | 0.00042 | 2.45 |

5Symbolic execution engine returns expressions with a lot of concatenations
A.4 Deobfuscation with Xyntia

We show in Section 7 that Xyntia bypasses state-of-the-art obfuscation strategies and enables to reverse VM handlers of program obfuscated with Tigress [11] and VMProtect [35]. We detail now (1) the obfuscation used in Section 7.1; (2) scripts to generate Tigress use cases from Section 7.2.

A.4.1 Effectiveness against usual protections. Section 7.1 shows that Xyntia enables to bypass usual protections. All tested obfuscation, except path-based obfuscation, were performed through Tigress [11]. Table 30 presents the Tigress commands used to generate obfuscated expressions. Conversely, evaluation of path based obfuscation relies on a custom encoding inspired from [26]. We present it now.

Path-based obfuscation [26, 36] takes advantage of the path explosion problem to thwart symbolic execution. While it is efficient against symbolic based analysis, what about blackbox ones? The example in Listing 2, is inspired by the For primitive from [26]. It computes the sum of x and y adding loops to increase the number of paths to explore (one path for each value of x and y), effectively killing symbolic execution. However, blackbox deobfuscation sees inputs-outputs behaviors only and would successfully synthesize the expression. To confirm it, we encoded B2 as in Listing 2. Table 4 shows the absence of impact.

```c
int sum(int x, int y){
    int x1, y1;
    for (int i = 0; i < x; i++){
        x1++;
    }
    for (int i = 0; i < y; i++){
        y1++;
    }
    return x1 + y1;
}
```

Listing 2: Sum function with path-oriented obfuscation

A.4.2 Virtualization based Deobfuscation. Section 7 shows that Xyntia enables to synthesize the VM-handler of software protected with Tigress [11] and VMProtect [35]. Table 31 presents the Tigress commands used to generate the 2 Tigress use cases (note that the "heavy_computing" function contains all mixed boolean-arithmetic expressions and is the one we want to obfuscate).

A.5 Counter AI-based deobfuscation : More details

Partial protections against blackbox deobfuscation methods have been discussed extensively in Section 8. We complete in the following (1) the description of the datasets used to evaluate the efficiency of the proposed methods; (2) the results of Syntia, CVC4 and STOKE against proposed protections.

A.5.1 Semantically complex handlers. Section 8.2 presents an encoding to translate a set of semantically simple handlers to complex ones. The proposed solution enables the creation of handlers as complex as wanted in terms of size and number of arguments. To evaluate the efficiency of the approach, we created 3 datasets namely BP1 (Table 34), BP2 (Table 35) and BP3 (too large to be presented here). Results of Xyntia, Syntia, CVC4 and STOKE-synth (STOKE-opti is not considered as it is not blackbox) are presented in Table 32. It confirms that the protection is highly effective.

A.5.2 Merged handlers. In Section 8.3, we measure the impact of conditionals on blackbox methods. We thus introduce 5 datasets containing 20 expressions each. The first one combines two basic handlers with one ITE, the second one combines 3 basic handlers though 2 nested conditionals and so on. The first and second datasets are given in Fig. 13. Each condition compares the third input (z) with a constant. The constant values are always sorted in increasing order starting from zero i.e., the first ITE compares z to 0, the second to 1, etc..

The results of Xyntia against merged handlers are presented in Section 8.3. We present now the evaluation of Syntia, CVC4 and STOKE-synth (STOKE-opti is not tested as it is not blackbox) on
the same datasets. Because we cannot change ITEs to the grammar of Syntia nor STOKE-synth, we evaluate them in their default configuration. Fig. 12 shows that in the utopian configuration CVC4 efficiently synthesizes all expressions with one conditional. However, we see that in any configuration, it is not able to synthesize expressions with nested conditionals. On the other hand, Table 33 shows that neither Syntia nor STOKE-synth is able to handle merged handler. Results confirm that merging handlers is an efficient protection, impeding sampling and synthesis.

Table 33: Syntia and STOKE-synth: Number of synthesized expressions against merged handlers (timeout = 60s)

|       | 1 | 2 | 3 | 4 | 5 |
|-------|---|---|---|---|---|
| Syntia| 0 | 0 | 0 | 0 | 0 |
| STOKE-synth| 0 | 0 | 0 | 0 | 0 |
### Table 34: Encoding of basic operators (BP1).

| Operator | Formula |
|----------|---------|
| **add**  | \( h_1 = (x + y) + -((a - x^2) - (xy)) \) |
|          | \( h_2 = (a - x^2) - xy + (-((y - (a \land x)) \times (y \land x))) \) |
|          | \( h_3 = (y - (a \land x)) \times (y \lor x) \) |
| **sub**  | \( h_1 = x - y - (xa - (y \lor a)) \) |
|          | \( h_2 = (xa - (y \lor a)) + -(((y \lor a) \times y) \times x) \) |
|          | \( h_3 = (((y \lor a) \times x) \times y) \times x \) |
| **mul**  | \( h_1 = x \times y + -(xa^2 - xy) \) |
|          | \( h_2 = xa^2 - xy + -(x \times y) - (a \times (x + y))) \) |
|          | \( h_3 = (x \times y) - (a \times (x + y)) \) |
| **and**  | \( h_1 = x \land y \land ((x \land a)^2 \lor y) \) |
|          | \( h_2 = ((x \land a)^2 \lor y) \times (ya - ((x \land a) + y)) \) |
|          | \( h_3 = ya - ((x \land a) + y) \) |
| **or**   | \( h_1 = x \lor y - (ya + x)^2 \) |
|          | \( h_2 = (ya + x)^2 + -(xa \times (y - (x \land a))) \) |
|          | \( h_3 = xa \times (y - (x \land a)) \) |

### Table 35: Encoding of basic operators (BP2).

| Operator | Formula |
|----------|---------|
| **add**  | \( h_1 = (x + y) + ((-(xy)^2) \land (-a \lor b)) - (x(d \land c)) \) |
|          | \( h_2 = -(((-(xy)^2) \land (-a \lor b)) - (x(d \land c))) + (((a - y \lor d) \land ((a - y \lor d) \land (c \land (d - x)))) \land (a \land (d - x)))) \) |
| **sub**  | \( h_1 = x - y + (((y \lor c) \times (x \land ((c \land (b^2)))) - (a + (b \land -d))) \land (a \land (b \land -d))) \) |
|          | \( h_2 = -(((y \lor c) \times (x \land ((c \land (b^2)))) - (a + (b \land -d))) \land (a \land (b \land -d))) + (((a - y \lor d) \land ((a - y - d)) \land (c \land (a \land x)))) \) |
|          | \( h_3 = -(((a - y \lor d) \land ((a - y - d)) \land (c \land (a \land x)))) \) |
| **mul**  | \( h_1 = (xy) \land (((y + -d) \land (x \land a)) \land (b \lor (c - a)))) \) |
|          | \( h_2 = (((y + -d) \land (x \land a)) \land (b \lor (c - a))) + (((a \land b) \land ((a \land b) \land (x \land y)))) \land (a \land c)) \) |
|          | \( h_3 = (((a \land b) \land ((a \land b) \land (x \land y)))) \land (a \land c)) \) |
| **and**  | \( h_1 = (x \land y) \land ((((x + d) \land (y \times ((b \land -a)))) \land (c \land b)) \land (-(d \land b) \land ((y \land b) \land (x \land c)))) \) |
|          | \( h_2 = ((((x + d) \land (y \times ((b \land -a)))) \land (c \land b)) \land (-(d \land b) \land ((y \land b) \land (x \land c)))) + (((d \land b) \land (y \land b) \land (x \land c)))) \) |
|          | \( h_3 = ((((d \land b) \land (y \land b) \land (x \land c)))) \) |
| **or**   | \( h_1 = (x \lor y) + (((((cd) \land (a \land b)) \land (a \land b)) \land (x \land -y))) \land c \) |
|          | \( h_2 = (((((cd) \land (a \land b)) \land (a \land b)) \land (x \land -y))) \land c) + (((c - (x \land b)) \land ((y \land (a \land y))) \land d) \land (x \land -c)) \) |
|          | \( h_3 = -(((c - (x \land b)) \land ((y \land (a \land y))) \land d) \land (x \land -c)) \) |
if $z = 0$ then $x + y$ else $x - y$
if $z = 0$ then $x + y$ else $x * y$
if $z = 0$ then $x + y$ else $x \land y$
if $z = 0$ then $x + y$ else $x \lor y$
if $z = 0$ then $x + y$ else $x \oplus y$
if $z = 0$ then $x - y$ else $x * y$
if $z = 0$ then $x - y$ else $x \land y$
if $z = 0$ then $x - y$ else $x \lor y$
if $z = 0$ then $x - y$ else $x \oplus y$
if $z = 0$ then $x - y$ else $x \land y$
if $z = 0$ then $x - y$ else $x \lor y$
if $z = 0$ then $x - y$ else $x \oplus y$
if $z = 0$ then $x * y$ else $x \land y$
if $z = 0$ then $x * y$ else $x \lor y$
if $z = 0$ then $x * y$ else $x \oplus y$
if $z = 0$ then $x \land y$ else $x + y$
if $z = 0$ then $x \land y$ else $x \lor y$
if $z = 0$ then $x \land y$ else $x \oplus y$
if $z = 0$ then $x \land y$ else $x - y$
if $z = 0$ then $x \land y$ else $x + y$
if $z = 0$ then $x \land y$ else $x - y$
if $z = 0$ then $x \land y$ else $x + y$

if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x * y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \land y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \lor y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \oplus y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \land y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \lor y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \oplus y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \land y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \lor y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \oplus y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \land y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \lor y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \oplus y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \land y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \lor y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \oplus y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \land y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \lor y$)
if $z = 0$ then $x + y$ else ( if $z = 1$ then $x - y$ else $x \oplus y$)

Figure 13: Merged handlers: datasets 1 and 2