Learning to Verify the Heap

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Abstract. We present a data-driven verification framework to automatically prove memory safety and functional correctness of heap programs. For this, we introduce a novel statistical machine learning technique that maps observed program states to (possibly disjunctive) separation logic formulas describing the invariant shape of (possibly nested) data structures at relevant program locations. We then attempt to verify these predictions using a theorem prover, where counterexamples to a predicted invariant are used as additional input to the shape predictor in a refinement loop. After obtaining valid shape invariants, we use a second learning algorithm to strengthen them with data invariants, again employing a refinement loop using the underlying theorem prover.

We have implemented our techniques in Cricket, an extension of the GRASShopper verification tool. Cricket is able to automatically prove memory safety and correctness of implementations of a variety of classical heap-manipulating programs such as insertionsort, quicksort and traversals of nested data structures.

1 Introduction

A number of recent projects have shown that it is possible to verify implementations of systems with complex functional specifications (e.g. CompCert \cite{compCert}, miTLS \cite{mTLS}, sel4 \cite{sel4}, and IronFleet \cite{ironFleet}). However, this requires highly skilled practitioners to manually annotate large programs with appropriate invariants. While there is little hope of automating the overall process, we believe that this annotation work could be largely automated. For this, we follow earlier work and infer likely invariants from observed program runs \cite{inferringInvariant1, inferringInvariant2, inferringInvariant3, inferringInvariant4, inferringInvariant5, inferringInvariant6, inferringInvariant7, inferringInvariant8}.

A key problem in verification of heap-manipulating programs is the inference of formal data structure descriptions. Separation logic \cite{separationLogic1, separationLogic2} has often been used in automatic reasoning about such programs, as its frame rule favors compositional reasoning and thus promises scalable verification tools. However, the resulting techniques have often traded precision and soundness for automation \cite{automation1}, required extensively annotated inputs \cite{extensivelyAnnotated1, extensivelyAnnotated2, extensivelyAnnotated3}, or focused on the restricted case of singly-linked lists (often without data) \cite{singlyLinked1, singlyLinked2, singlyLinked3, singlyLinked4, singlyLinked5, singlyLinked6, singlyLinked7}.

At its core, finding a program invariant is searching for a general “concept” (in the form of a formula from an abstract domain) that overapproximates all occurring program states. This is similar to many of the problems considered in statistical machine learning, and recent results have shown that program analysis questions can be treated as such problems \cite{statisticalMachineLearning1, statisticalMachineLearning2, statisticalMachineLearning3, statisticalMachineLearning4, statisticalMachineLearning5}. With the exception of \cite{statisticalMachineLearning6, statisticalMachineLearning7}, these efforts have focused on numerical program invariants.
We show how to treat the prediction of formulas similarly to predicting natural language or program source code in Sect. 3. Concretely, we define a simple grammar for our abstract domain of separation logic formulas with (possibly nested) inductive predicates. Based on a set of observed states, a formula can then be predicted starting from the grammar’s start symbol by sequentially choosing the most likely production step. As our grammar is fixed, each such step is a simple classification problem from machine learning: “Considering the program states and the formula produced so far, which is the most likely production step?” Our technique can handle arbitrary (pre-defined) inductive predicates and nesting of such predicates, and can also produce disjunctive formulas.

We show how to use this technique in a refinement loop with an off-the-shelf program verifier (GRASShopper [35]) to automatically prove memory safety of programs in Sect. 4. We add a second refinement loop integrating numerical invariants into the predicted shape invariants in Sect. 5, adapting a technique developed for functional programming [43]. Finally, we combine everything in our tool Cricket and experimentally evaluate it in Sect. 6, showing that it can fully automatically verify programs that are beyond the capabilities of other tools.

Limitations. As we rely on the underlying program verifier to check correctness of our invariant predictions, we “inherit” its C-like “simple programming language” (SPL). Furthermore, our performance depends on that of the underlying verifier, and in fact, time spent in GRASShopper dominates our implementation’s runtime. As our technique relies on observing a sample of occurring program states, it is sensitive to the choice of initial samples (randomly sampled, taken from a test suite, or provided by a human) used in the sample collection phase. Finally, our two-step approach (first shape, then arithmetic invariants) is not able to reason about programs whose memory safety depends on arithmetic arguments, e.g., examples in which memory safety depends on two lists having the same length.

Related Work. Memory safety proofs have long been a focus of research, and we only discuss especially recent and close work here, and compare our implementation with some tools in Sect. 6. (Bi)-abduction based shape analyses [10–12,25,26] have been used successfully in memory safety proofs, and can also be used to abduce needed preconditions or the required inductive predicates. In another recent line of work, forest automata have been used to verify heap-manipulating programs [1], but require hard-coded support for specific data structures.

In property-directed shape analysis [21], predicate abstraction over user-provided shape predicates (sorted list segments, . . . ) is combined with a variation of the IC3 property-directed reachability algorithm [8] to prove memory safety and data properties. This can be viewed as continuation of three-valued logic-based works (e.g. [37]), reducing the data type specification requirements. Similarly, SplInter extends the Impact [30] safety prover with heap reasoning based on an interpolation technique for separation logic. While we could not obtain working copies of the implementations, the reported results indicate that they cannot prove correctness of more advanced examples such as sorting algorithms.

Closest to this work is [32] which infers likely heap invariants from program traces (i.e., it infers shapes from usage patterns) using machine learning techniques. However, it is not able to reason about data in these data structures.
procedure insert (lst : Node, elt : Node) returns (res : Node)

ensures \( \text{lseg}(\text{res}, \text{null}) \) & \( \text{slseg}(\text{res}, \text{null}) \rightarrow \text{null} \}

\[
\text{if } (\text{lst} == \text{null} \text{ or } \text{lst}.\text{data} > \text{elt}.\text{data}) \{
\text{elt}.$next$ := \text{lst} ;
\text{return elt} ;
\} \text{ else } \{
\text{var cur} := \text{lst} ;
\text{while} (\text{cur}.$next$ == \text{null} \text{ or } \text{cur}.$next$.\text{data} < \text{elt}.$data$)
\text{invariant } \begin{cases}
\text{cur} != \text{null} & \& \text{elt} != \text{null} & \& \text{lseg}(\text{lst}, \text{cur}) & \& \text{slseg}(\text{cur}, \text{null}) & \& \text{slseg}(\text{elt}, \text{null})
\text{cur}.$next$ := \text{cur}.$next$ ;
\text{elt}.$next$ := \text{cur}.$next$ ;
\text{cur}.$next$ := \text{elt} ;
\text{return lst} ;
\end{cases}
\}
\]

Fig. 1: Procedure inserting element into a sorted list. Inferred shape (resp. shape-
data) loop invariants and postconditions are shown in a box (resp. dashed box).

2 Example

We demonstrate the key points of our method on a simple example. The program in Fig. 1 is taken from the GRASShopper test suite, and our goal is to automatically infer a loop invariant and postcondition.

The program operates on singly-linked lists where list elements are Nodes with a next and a data field, and inserts a given element into the correct position of a sorted list. So if lst is [2, 4, 6, 9] (a list containing the elements 2, 4, 6, and 9) and elt is the singleton list [7], insert modifies lst such that it is [2, 4, 6, 7, 9]. The separating conjunction from separation logic is written as \( \& \& \) and elt.$next$ \( \rightarrow \) null indicates that (i) elt.$next$ is null and that (ii) elt is non-null. Without an explicit loop invariant, GRASShopper cannot prove memory safety nor correctness.

Shape Invariants. First, we prove memory safety using only shape properties. We sample program states satisfying the preconditions slseg(lst, null) \( \& \& \) elt.$next$ \( \rightarrow \) null, obtaining states such as the one at the top of Fig. 2, where a node is a heap cell, data is displayed in it, and next pointers are shown as edges. We then execute the program on these states and record execution states at the head of the while loop to obtain a set of reachable program states \( S^+ \) (displayed in Fig. 2 below the line).

The set \( S^+ \) is then passed to our shape invariant predictor Platypus. Platypus predicts a separation logic formula by following its syntactic structure (i.e., it predicts a syntax tree top-down). Thus, formula prediction reduces to predicting a sequence of single production steps. Each such step has a simple intuitive meaning, e.g., which data structure is used in a part of a heap graph, or at which variable such a data structure starts. These predictions are implemented using standard tools from statistical machine learning, based on features extracted from the

\[\text{(ii) follows implicitly from the statement about one of elt's fields.}\]
observed program states and the partial formula predicted so far. For our example, we predict \( \text{lseg}(\text{lst}, \text{cur}) \land \text{lseg}(\text{cur}, \text{null}) \land \text{lseg}(\text{elt}, \text{null}) \). A standard nullness analysis additionally yields \( \text{cur} \neq \text{null} \land \text{elt} \neq \text{null} \) and leads to the loop invariant shown in Fig. 1, which we ask GRASShopper to verify for the program. The postcondition \( \text{lseg}(\text{res}, \text{null}) \) is inferred similarly.

This proof succeeds, and thus we have proven memory safety of the program. If the proof had failed, a counterexample state would have been returned, which would be used as additional input for Platypus to produce a more precise invariant.

**Shape/Data Invariants.** In a second step, we strengthen the obtained memory safety proof to prove functional correctness of our program. We use the same samples that we used to predict the shape invariants above, splitting the observed data into different groups according to the inferred shape predicates, and infer data invariants on these groups. The data for different components (observed lists and data fields of structs referenced directly by stack variables) is shown in Fig. 3. Following [43], we use the observed data to learn quantified invariants.

<table>
<thead>
<tr>
<th>State element</th>
<th>Iter. 1</th>
<th>Iter. 2</th>
<th>Iter. 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{lseg}(&lt;\text{lst}, \text{cur}&gt;) )</td>
<td>[]</td>
<td>[2]</td>
<td>[2,4]</td>
</tr>
<tr>
<td>( \text{lseg}(\text{cur}, \text{null}) )</td>
<td>[2,4,6,9]</td>
<td>[4,6,9]</td>
<td>[6,9]</td>
</tr>
<tr>
<td>( \text{lseg}(\text{elt}, \text{null}) )</td>
<td>[7]</td>
<td>[7]</td>
<td>[7]</td>
</tr>
<tr>
<td>( \text{lst}.\text{data} )</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>( \text{cur}.\text{data} )</td>
<td>2</td>
<td>4</td>
<td>6</td>
</tr>
<tr>
<td>( \text{elt}.\text{data} )</td>
<td>7</td>
<td>7</td>
<td>7</td>
</tr>
</tbody>
</table>

Fig. 3: Data of \( \text{insert} \) on \( [2,4,6,9] \).

For this, we use the footprint \( \text{FP} \) of a separation logic predicate, e.g., \( \text{FP}(\text{lseg}(\text{lst}, \text{cur})) \) contains the Node objects in the list between \( \text{lst} \) and \( \text{cur} \). We define a containment predicate \( u \in \text{FP}(\text{lseg}(\text{lst}, \text{cur})) \) to check whether a node \( u \) is in the footprint, and an ordering predicate \( \text{FP}(\text{lseg}(\text{lst}, \text{cur})) : u \rightarrow^+ v \) which is true iff \( v \) can be reached from \( u \) by repeated dereference in the footprint (these predicates are similar to those used in [21]).

We infer universally quantified arithmetic invariants with quantifiers ranging over the footprints of the considered list segments using our observations. In our case, this yields \( \forall u. u \in \text{FP}(\text{lseg}(\text{lst}, \text{cur})) \Rightarrow u\.\text{data} \leq \text{cur}\.\text{data} \), reflecting that every element of the list from \( \text{lst} \) to \( \text{cur} \) only contains elements smaller than \( \text{cur}\.\text{data} \). Similarly, we also find \( \forall u, v. \text{FP}(\text{lseg}(\text{lst}, \text{cur})) : u \rightarrow^+ v \Rightarrow u\.\text{data} \leq v\.\text{data} \), \( \forall u, v. \text{FP}(\text{lseg}(\text{cur}, \text{null})) : u \rightarrow^+ v \Rightarrow u\.\text{data} \leq v\.\text{data} \), reflecting sortedness in these footprints, and \( \text{cur}\.\text{data} \leq \text{elt}\.\text{data} \). In Fig. 1 we denote this by using \( \text{lseg} \) for sorted list segments and \( \text{lsseg}(x, y, v) \) for a sorted list segment from \( x \) to \( y \) whose values are bounded by \( v \). After strengthening the loop invariant obtained before with this information, GRASShopper can prove that the postcondition of \( \text{insert} \) shown in Fig. 1 always holds.

## 3 Predicting Shape Invariants from Heaps

In this section, we first discuss a general technique to predict derivations in a grammar \( G \) from a set of objects \( \mathcal{H} \), given functions that compute features from \( \mathcal{H} \). We then show how to apply this to our setting, using separation logic as language and heap graphs as input objects, and discuss the used features. Finally, we discuss some extensions that were useful for our implementation Platypus.
3.1 General Parse Tree Prediction

Let $G$ be a context-free grammar, $S$ the set of all (both terminal and nonterminal) symbols of $G$, and $N$ just the nonterminal symbols. We aim to learn how to predict parse trees in $G$, following a similar technique that predicts source code from natural language [2]. We represent parse trees as tuples $T = (A, g(\cdot), ch(\cdot))$ where $A = \{1, \ldots, A\}$ is the set of nodes for some $A \in N$, $g : A \rightarrow S$ maps a node to a terminal or nonterminal node from the grammar, and $ch : A \rightarrow A^*$ maps a node to its direct children in the syntax tree. A partial parse tree $T_{<a}$ is a parse tree $T$ restricted to nodes $\{1, \ldots, a - 1\}$, where the ordering on nodes comes from the order in which they are predicted (see below).

We formulate the algorithm as a sequential prediction task where we predict the parse tree in a depth-first left-to-right node order. Each prediction step is conditional upon all of the predictions that have been made so far, and corresponds to picking a production rule from $G$ to expand the current nonterminal $N \in N$. To make these predictions, we extract a feature vector $\phi_N(\hat{H}, T_{<a}) \in \mathbb{R}^{D_N}$ (where $D_N$ is the number of features for $N$) that depends on the considered nonterminal $N$, the input objects $\hat{H}$ and the partial syntax tree $T_{<a}$ generated so far.

Depending on the kind of production rules we have to expand $N$, we can then view this either as a multiclass classification task (if there is a fixed, small number of productions) or as a ranking task (if the production requires us to pick from a set of terminals that are not fixed at training time, such as program variables). A standard machine learning algorithm can then be used on the computed features to make a prediction. In practice, we use logistic regression for all classification tasks and a simple two-layer neural network for the ranking tasks. The pseudocode for this procedure PlatypusCore is given in Alg. 1, which is initially called with a parse tree containing only the grammar’s start symbol. The probability of a full parse tree $T$ can be expressed as the product of probabilities of the individual production choices, i.e., $p(T | \hat{H}) = \prod_{a \in A \mid g(a) \in N} p(ch(a) | \hat{H}, T_{<a})$.

Algorithm 1: Pseudocode for PlatypusCore (extension of [2])

Input: Grammar $G$, input objects $\hat{H}$, (partial) parse tree $T = (A, g, ch)$, nonterminal node $a$ to expand

1: $N \leftarrow g(a)$ \hspace{1cm} \{nonterminal symbol of $a$ in $T$\}
2: $\phi \leftarrow \phi_N(\hat{H}, T)$ \hspace{1cm} \{compute features (see Sect. 3.2)\}
3: $P \leftarrow$ most likely production $N \rightarrow S^+$ from $G$ considering $\phi$
4: $T \leftarrow$ insert new nodes into $T$ according to $P$
5: for all children $a' \in ch(a)$ labeled by nonterminal do
6: $T \leftarrow$ PlatypusCore($G, \hat{H}, T, a'$)
7: return $T$

To train the overall system, we process input sets $\hat{H}$ with their corresponding ground truth parse tree $T$ to obtain pairs $(\phi^{g(a)}(\hat{H}, T_{<a}), P)_{a \in A}$ of feature vectors and chosen production rules $P$. For this, we follow the parse tree structure analogously to Alg. 1, at each step extracting the feature vector and the chosen ground truth production rule. We then use the extracted data as training data for the individual classifiers and rankers.
3.2 Predicting Separation Logic Formulas

**Inputs** Our inputs are directed, possibly cyclic, graphs representing the heap of a program and the values of program variables. Intuitively, each graph node $v$ corresponds to an address in memory at which a sequence of pointers $v_0, \ldots, v_t$ is stored.\(^7\) Edges reflect these pointer values, i.e., $v$ has edges to $v_0, \ldots, v_t$ labeled with $0, \ldots, t$. The node 0 is special (corresponding to the null pointer in programs) and may not have outgoing edges. Furthermore, we use unique node labels to denote the values of program variables $PV$ and auxiliary variables $V$.

**Definition 1 (Heap Graphs).** Let $PV$ be a set of program variables. The set of Heap Graphs $HG$ is then defined as $2^N \times 2(\{0\})^N \times (PV \cup V \to \mathbb{N})$.

**Outputs** We consider a fragment of separation logic [33, 36]. Our method allows the separating conjunction $\&$, list-valued points-to expressions $v \mapsto [e_1, \ldots, e_n]$, existential quantification and higher-order inductive predicates [5], but no $\neg$. As pure formulas, we only allow conjunctions of (dis)equalities between identifiers, and use the constant 0 as the special null pointer. We will only discuss the singly-linked list predicate $ls$ and the binary tree predicate $tree$ in the following, though our method is applicable to generic inductive predicates. Given a set of fresh variables $V$, the following grammar describes our formulas:

\[
\varphi := \exists V, \varphi \mid II : \Sigma \quad \Sigma := \text{emp} \mid \sigma \ast \Sigma \quad \sigma := \text{ls}(E, E, E, V, V \to \varphi) \mid \text{tree}(E, E, V, V, V \to \varphi) \\
II := \text{true} \mid \pi \land II \quad \pi := E = E \mid E \neq E \\
E := 0 \mid \varphi \mid V \mid PV \\
V := [E \ldots E] \mid PV \mapsto [E \ldots E]
\]

Semantics are defined as usual for separation logic, i.e., $\hat{H} \models \sigma_1 \ast \sigma_2$ for some $\hat{H} = (V, E, L) \in HG$ if $\hat{H}$ can be partitioned into two subgraphs $\hat{H}_1, \hat{H}_2$ such that $\hat{H}_1$ (resp. $\hat{H}_2$) is a model of $\sigma_1$ (resp. $\sigma_2$) after substituting variables in $\sigma_1$ and $\sigma_2$ according to $L$. The empty heap $\text{emp}$ is true only on empty subgraphs, and $v \mapsto [e_1, \ldots, e_n]$ holds iff for all $1 \leq i \leq n$, there is some edge $(v, i, e_i)$. For detailed semantics, we refer to [33, 36]. The semantics of inductive predicates are the least fixedpoint of their definitions, where nested formulas describe the shape of a nested data structure. For example, $ls$ and $tree$ are defined as follows:

\[
\begin{align*}
\text{ls}(x, y, \varphi) &\equiv (x = y) \lor (\exists n, n.x \mapsto [v, n] \ast \text{ls}(n, y, \varphi) \ast \varphi(x, y, v, n)) \\
\text{tree}(x, \varphi) &\equiv (\exists v, l, r, l \neq 0 \land r \neq 0; x \mapsto [v, l, r] \ast \text{tree}(l, \varphi) \ast \text{tree}(r, \varphi) \ast \varphi(x, v, l, r)) \\
&\quad \lor (\exists x, r.h \neq 0; x \mapsto [v, 0, r] \ast \text{tree}(r, \varphi) \ast \varphi(x, v, 0, r)) \\
&\quad \lor (\exists v, l, l \neq 0; r \mapsto [v, l, 0] \ast \text{tree}(l, \varphi) \ast \varphi(v, x, l, 0)) \\
&\quad \lor (\exists v, x \mapsto [v, 0, 0] \ast \varphi(x, v, 0, 0))
\end{align*}
\]

We use $\top \equiv \lambda v_1, v_2, v_3, v_4 \to \text{true} : \text{emp}$ to denote “no further nesting”. Thus, $\text{ls}(x, y, \lambda f_1, f_2, e_1, e_2 \to \text{tree}(e_1, \top))$ describes a list of binary trees from $x$ to $y$.

**Example 2.** A “pan-handle list” starting in $i_2$ is described by $\varphi(i_2, i_2, i_3, i_4) \equiv \exists t. \text{ls}(i_2, t, \top) \ast \text{ls}(t, t, \top)$, where an acyclic list segment leads to a cyclic list. Here, $t$ is the existentially quantified node at which “handle” and “pan” are joined.

\(^7\) In this section, we discard non-pointer values.
The formula $\psi(x) \equiv \text{tree}(x, \varphi)$ describes a binary tree whose nodes in turn contain panhandle lists. An example of a heap satisfying the formula $\psi$ is shown in Fig. 4. Blue nodes are elements of the tree data structure, having three outgoing edges labeled 0, 1, 2. Each of the green boxes in Fig. 4 corresponds to a subheap that is described by the subformula $\varphi$. In each of these subheaps, one node (where the “handle” of a panhandle list meets the “pan”) is labeled with $t$ – note that $t$ is not a program variable, but introduced through the existential quantifier in $\varphi$.

We found that our procedure PlatypusCore was often imprecise when generating the pure subformula $\Pi$ and $\mapsto$ atoms. For this reason, we generate $\Pi$ deterministically with a nullness analysis (see Sect. 3.3), and completely omit $\mapsto$. Our grammar thus simplifies as follows (where $\Pi$ is now a terminal symbol).

$$
\varphi ::= \exists V. \varphi \mid \Pi : \Sigma \\
\Sigma ::= \text{emp} \mid \sigma \ast \Sigma
$$

$$
E ::= 0 \mid V \mid PV \\
\sigma ::= \text{ls}(E, E, \lambda V, V, V \rightarrow \varphi) \mid \text{tree}(E, \lambda V, V, V \rightarrow \varphi)
$$

### Predicting Flat Formulas

We first consider the case where the input is a single graph $\hat{\mathcal{H}}$ with nodes $V$, and predict formulas from a restricted separation logic grammar without nesting. These two restrictions are connected, as we treat nested data structures by considering each “subheap” as an additional input (see below). We will discuss the construction of $\phi^N$ for this simple case first.

For any $a$, we define $I(T_{<a})$ as the set of identifiers that are in scope at point $a$ in the partial parse tree, and $D(T_{<a}) \subseteq I(T_{<a})$ as the set of “defined” identifiers that occur in the first argument of $\text{ls}$ and $\text{tree}$ predicates (i.e., whose corresponding data structure has already been predicted). We use this to compute features useful for predicting the expansion of an $E$ nonterminal into an identifier.

An important class of features is based on the notion of $n$-grams of heap graph paths. Each node $v$ is identified with a 1-gram: A pair $(\text{indeg}(v), \text{outdeg}(v)) \in \mathbb{N}^2$ corresponding to its in- and outdegree. A 2-gram is a pair of the 1-grams for two nodes connected by an edge in $\hat{\mathcal{H}}$. Based on this, we define a measure of depth. For a path $v_1 \ldots v_t$ in the heap graph, we define its 1-gram depth as the number of times the 1-gram changes, i.e., $|\{i \in \{1 \ldots t - 1\} \mid \text{indeg}(v_i) \neq \text{indeg}(v_{i+1}) \lor \text{outdeg}(v_i) \neq \text{outdeg}(v_{i+1})\}|$. Then, $\text{depth}(v)$ is the minimal depth of paths leading from a node labeled by a variable to $v$. In our method, we extend 1-grams by this depth notion, i.e., represent each node by a $(\text{indeg}(v), \text{outdeg}(v), \text{depth}(v))$ triple. Intuitively, this information helps to discover the level of data structure nesting.

To extract features from a heap graph, we count the number of occurrences of an n-gram in that graph, only considering the n-grams observed at training time.

As an example, consider Fig. 4 again. There, node 1 has 1-gram depth 0, nodes 3, 4, and 13 have 1-gram depth 1 (note that we haven’t drawn the edges to 0 for some “tree” nodes), and nodes 8, 9, 2, 11 and 14 have 1-gram depth 2. Thus for the whole graph, we compute the 1-gram features $1\text{gram}_{(0,3,0)} = 1$ (for node 1), $1\text{gram}_{(1,3,1)} = 3$ (for nodes 3, 4, and 13) and so on.
Features for $\Sigma$, $\sigma$ Nonterminals Intuitively, the $\Sigma$ production step depends on whether the syntax tree generated so far “explains” the observed heap graphs, or if further headets are needed. In the $\sigma$ production step, the right predicate (i.e., either $\mathsf{ls}$ or $\mathsf{tree}$) needs to be picked. To this end, we use a simple procedure that approximates the footprint of the syntax tree generated so far, denoted $V_{<a}$ for some syntax tree node $a$. We then compute 1- and 2-gram features from above restricted to the nodes $V \setminus V_{<a}$, i.e., those nodes that are not covered by the data structures described by the partial formula predicted so far. Their node counts, contained in the 1-gram features, are indicators of the data structures that have not been predicted yet.

Let $I_{<a} = I(\mathcal{T}_{<a}) \setminus \mathcal{D}(\mathcal{T}_{<a})$ be the identifiers that are in scope, but have not appeared in the first position of a predicate. We compute n-gram features restricted to $V|_{I_{<a}} \setminus V_{<a}$, where $V|_{I_{<a}}$ denotes the nodes in $\mathcal{H}$ reachable from $I_{<a}$. Note that we use fresh names for all $V$ bound by $\lambda$ in the $\sigma$ production rules.

Features for $E$ Nonterminals Here, we pick an expression as argument to a predicate. When making a prediction for $E$ at node $a$, the set of legal outputs is $I(\mathcal{T}_{<a}) \cup \{0\}$; i.e., the set of all identifiers that are in scope at this point and 0.

To handle this, we compute one feature vector $\phi^E_v$ for each $z \in I(\mathcal{T}_{<a}) \cup \{0\}$, based on connectivity to other graph nodes. Intuitively, we need to find the “start” of a data structure (i.e., $\mathsf{tree}(x)$) or something reachable from the start (i.e., $y$ in $\mathsf{ls}(x, y)$). For this, we define the sequence of “enclosing defined identifiers” $e_1, \ldots, e_t \in I(\mathcal{T}_{<a})$, i.e., identifiers appearing in predicates enclosing the currently considered node $a$. As an example, consider the partially predicted formula $\mathsf{ls}(x, y, \lambda i_1, i_2, i_3, i_4 \to \mathsf{ls}(v, \ldots))$, where we are interested in predicting the expression at $z$. Here, we have $e_1 = v$ and $e_2 = x$. We use one boolean feature to denote reachability of (resp. from) each $e_1, \ldots, e_t$ from (resp. of) $z$.

To make a prediction, we use a neural network $\mathsf{NN}$ (with learnable parameters $\theta^E$) to compute a score $s_z = \mathsf{NN}(\phi^E_v; \theta^E)$. The probability of $z$ is then computed via a softmax, i.e., $p(z) = \frac{\exp(s_z)}{\sum_{z' \in I(\mathcal{T}_{<a}) \cup \{0\}} \exp(s_{z'}),}$

Features for $\varphi$ Nonterminals Here, we need to decide whether to declare new identifiers via existential quantification, so that we can later refer back to them (e.g., for panhandle lists). We found it advantageous to not only predict that we need a quantifier, but also by which graph node it should be instantiated.

We proceed similar to the $E$ case and compute a feature vector $\phi^\varphi_v$ for each node $v \in \mathcal{H}$. Features are standard graph properties, such as membership in a strongly connected component, existence of labels for a node, and the 1- and 2-gram features discussed above. We use a neural network $\mathsf{NN}$ (with learnable parameters $\theta^\varphi$) to compute a score $s_v = \mathsf{NN}(\phi^\varphi_v; \theta^\varphi)$. The output is passed through a logistic sigmoid to give the probability that a new identifier, corresponding to node $v$ in the heap graph, should be instantiated. When choosing a production for $\varphi$, we thus make independent predictions for each $v$ and instantiate a fresh identifier $i_v$ for each $v$ that was predicted to be “on”.

---

8 For $p(v, v_1, \ldots, v_n)$, we compute the footprint approximation as all those heap nodes reachable via recursive fields used in the definition of $p$ without passing nodes $v_1 \ldots v_n$. See Sect. 6.2 for how to instead learn this approximation.
Predicting Nested Formulas In the general case we have several input heap graphs \( \mathcal{H} \), and data structures may in turn contain other data structures. This requires us to make predictions that are based on the information in all graphs, and sometimes on several subgraphs of each of the graphs. As an example, consider again the heap in Fig. 4, and imagine that we have successfully predicted the outer part of the corresponding formula, i.e., \( \text{tree}(x, \lambda i_1, i_2, i_3, i_4 ?) \), and are now trying to expand \( ? \). This subformula needs to describe all the subheaps corresponding to the contents of the green boxes in Fig. 4. To handle this, we now allow modifying the input \( \mathcal{H} \) after a production step (between line 4 and 5 of PlatypusCore). So for our example, we would change \( \mathcal{H} \) to contain one heap graph with labels \( \{x \mapsto 1, i_1 \mapsto 3, i_2 \mapsto 8, i_3 \mapsto 0, i_4 \mapsto 0\} \) for the leftmost box, one with labels \( \{x \mapsto 1, i_1 \mapsto 1, i_2 \mapsto 2, i_3 \mapsto 3, i_4 \mapsto 4\} \) for the second box, and so on.

Everything but \( \varphi \) Nonterminals We directly lift the techniques from Sect. 3.2. The main difference is that we now have to handle a set of heap graphs \( \hat{\mathcal{H}} \). We compute feature vectors for each heap graph independently as before, and then merge them into a new single feature vector by computing features based on the maximum \( f_{\text{max}} \), minimum \( f_{\text{min}} \), and average value \( f_{\text{avg}} \) of each feature \( f \).

\( \varphi \) nonterminals This covers the prediction of \( \exists t \), where \( t \) corresponds to one node in each of the green boxes in Fig. 4. As the number of nodes may differ between the different heap graphs, we cannot simply lift our technique from above.

This problem is a basic form of the structured prediction problem [4]. Suppose there are \( R \) heap graphs. For each of the graphs, there is a set of nodes \( V_r \) which may require an existential quantifier to be described in our setting (in Fig. 4, these are the contents of the green boxes). Let \( y_v \) be a boolean denoting the event that a new identifier is declared for node \( v \). We train a neural network like in the single-heap case so that the probability of declaring a variable for node \( v \) is \( p(y_v = 1) = \frac{1}{1 + \exp -s_v} \), where \( s_v \) is the score output by the NN. To make predictions, we set the probabilities of illegal events to 0 and then predict using the distribution over the remaining possibilities. Letting \( Z_r = \prod_{v \in V_r} \left(1 + \exp -s_v \right) \), the probability of not declaring any variables is \( \prod_r \prod_{v \in V_r} (1 - p(y_v = 1)) = \prod_r \frac{1}{Z_r} \). The probability of selecting exactly node \( v \) from subheap \( r \) is \( \frac{1}{Z_r} \prod_{v \in V_r, v' \neq v} \frac{1}{1 + \exp -s_v} \). As the choice of node from each subheap is independent given that we are declaring a new identifier, the probability of choosing the set of nodes \( \{v_r\} \), is the product \( \prod_r \frac{1}{Z_r} \). Noting that all legal joint configurations have the same denominator \( \prod_r Z_r \), we can drop the denominator and compute the normalizing constant for the constrained space later. The total unnormalized probability of declaring a variable is the sum of the unnormalized probabilities of all ways to choose one \( v_r \) from each subheap \( r \), which can be written as \( \prod_r \sum_{v \in V_r} \exp s_v \).

To make predictions, we compute the set of scores \( s_r = \{s_v \mid v \in V_r\} \). We first decide whether to declare a new identifier. Following from above, the probability of not declaring a new identifier is \( \frac{1 + \prod_r \sum_{v \in V_r} \exp s_v}{\prod_r \sum_{v \in V_r} \exp s_v} \) while the probability of declaring a new identifier is \( \frac{\prod_r \sum_{v \in V_r} \exp s_v}{\prod_r \sum_{v \in V_r} \exp s_v} \). To make a prediction under these constraints, we can first compute the probability that a new identifier is declared in each subheap. If we decide not to declare a variable, we instead choose the \( \Pi : \Sigma \) production. If we decide to declare a variable, then we draw one node
from each subheap according to a softmax over the scores; i.e., the probability of choosing node \( v \) in subheap \( r \) is \( \frac{\exp s_v}{\sum_{v' \in V_r} \exp s_{v'}} \). Similar reasoning can be applied to find the most likely configuration of \( y_v \) variables to make a prediction.

### 3.3 Predictions with Platypus

As discussed above, we have separate procedures to produce pure subformulas and to generate disjunctive formulas. Furthermore, we have adapted PlatypusCore to not only greedily select the most likely production rule at each step, but to sample several invariant candidates, returned in order of their respective probability.

**Pure Subformulas** We use a deterministic procedure to expand the nonterminal \( \Pi \) describing the pure part of our formulas, using a simple aliasing and nullness analysis. Namely, for all pairs of identifiers \( x, y \in PV \cup \{0\} \), we check if \( x = y \) or \( x \neq y \) holds in all input heap graphs. \( \Pi \) is then set to the conjunction of all equalities that hold in all inputs graphs.

**Handling Disjunctions** We found disjunctive separation logic formulas to be needed even for surprisingly simple examples, as in many cases, the initial or final iteration of a loop requires a (slightly) different shape description from all other steps. In our setting, the problem of deciding how many and what disjuncts are needed can be treated as a clustering problem of heap graphs. As features, we use booleans indicating reachability between program variables as above. As clustering algorithm, we use standard \( k \)-means clustering, using the Euclidean distance between feature vectors as heap graph distance. In our implementation, we run the clustering algorithm for \( k \in 1..4 \) and use the clustering that results in the formula with highest probability according to our formula predictor.

**Generating Training Data** Training the logistic regressors and neural nets from above requires large amounts of training data, i.e., heap graphs labeled with corresponding formulas. To obtain this data, we fix program variables \( PV \) and enumerate derivations of formulas in our grammar, similar in spirit to [23]. For each of the generated formulas, we enumerate models by expanding inductive predicates until only \( \to \) atoms remain. From this we read off heap graphs by resolving the remaining ambiguous possible equalities between variables.

### 4 Refining and Verifying Shape Invariants

We construct our fully automatic memory safety verifier Locust (pseudocode in Alg. 2) by connecting our shape predictor from Sect. 3 with the program verifier GRASShopper. For this, we keep a list of positive \( S^+(\ell) \) and negative state samples \( S^-(\ell) \) for every program location \( \ell \) at which program annotations for GRASShopper are required (i.e., loop invariants and pre/post-conditions for subprocedures). We collect an initial set of positive samples by simply executing the program. Then we obtain a set of candidate formulas from Platypus for each location and enter a refinement loop. If verification using these candidates fails, GRASShopper returns a counterexample state at some location \( \ell \), which we use to extend the sets \( S^+(\ell) \) and \( S^-(\ell) \). If no counterexample is returned, soundness of GRASShopper implies memory safety. It is possible that no correct set of program

\[9\] In practice, this set is so large that we only sample from it.
Algorithm 2 Pseudocode for Locust

Input: Program \( P \) and entry procedure \( p \) with precondition \( \varphi_p \), locations \( L \) requiring program annotations

1. \( I \leftarrow \) sample initial states satisfying \( \varphi_p \) \{see Sect. 4.1\}
2. \( S^+ \leftarrow \) execute \( P \) on \( I \) to map location \( \ell \in L \) to set of observed states
3. \( \textbf{while true do} \)
4. \( \textbf{for all } \ell \in L \textbf{ do} \)
5. \( \varphi_1^\ell, \ldots, \varphi_k^\ell \leftarrow \) obtain \( k \) candidates from Platypus\((S^+(\ell))\)
6. \( \varphi_\ell \leftarrow \) first \( \varphi_i^\ell \) proven consistent with all \( S^+(\ell), S^-(\ell) \) \{see Sect. 4.3\}
7. \( P' \leftarrow \) annotate \( P \) with inferred \( \varphi_\ell \)
8. \( \textbf{if } \mathtt{GRASShopper}(P') \text{ returns counterexample } s \text{ then} \)
9. \( \quad \textbf{if } s \text{ is new counterexample then} \)
10. \( \quad \text{update } S^+, S^- \text{ to contain } s \text{ for correct location} \) \{see Sect. 4.2\}
11. \( \quad \textbf{else return FAIL} \)
12. \( \textbf{else return SUCCESS} \)

To simplify the procedure, we assume that Platypus always returns the most precise formula from our abstract domain holding for the given set of input heap graphs \( (\dagger) \). While this is not guaranteed, the system was trained to produce this behavior, and we observe that our implementation behaves like this in practice.

4.1 Initial State Sampling

We assume the existence of some set of preconditions describing the input to the main procedure of the program in separation logic.\(^{10}\) To sample from these preconditions, we can add \texttt{assert false} to the beginning of the program. Then, every counterexample returned by \texttt{GRASShopper} is a model of the precondition. To get more samples, and to ensure different sizes of input lists, we add cardinality constraints to the precondition. For example, to force a list starting at \texttt{lst} to have length \( \geq 3 \), we add \texttt{requires lst.next.next != null}. States at other locations are then obtained by executing the program from the initial sample.

While this strategy is complete relative to the fragment of separation logic supported by \texttt{GRASShopper}, it is slow even for simple preconditions. Thus, in practice, we use a simple heuristic sampling algorithm for simple preconditions (without arithmetic constraints), and generate sample states of varying sizes.

4.2 Handling Counterexamples

If the program is incorrect, or the current annotations are incorrect or insufficient to prove the program correct, then \texttt{GRASShopper} returns a counterexample at a location \( \ell \). Depending on the context of such a counterexample and its exact form, we treat it as a positive or negative program state sample as follows.

– Case 1: A candidate invariant does not hold on loop entry. The counterexample state is reachable, but is not covered by the candidate loop invariant, and thus, the counterexample can be added as a positive sample to \( S^+(\ell) \).

\(^{10}\) Conceivably, these could be provided by users in a pre-formal language and translated to separation logic using an interactive elaboration procedure. Alternatively, given a test suite, Platypus could predict the initial precondition as well.
– Case 2: A candidate loop invariant is not inductive. This is an implication counterexample [15,40], i.e., a state \( s \) that is a model of the candidate loop invariant and a state \( s' \) reached after evaluating the loop body on \( s \). Based on our assumption (†), we conclude that \( s \) is likely to be a reachable state, and thus \( s' \) is. Hence, we treat \( s' \) as a positive sample and add it to \( S^+(\ell) \).
– Case 3: A postcondition does not hold for a state \( s \). Again, by (†), we conclude that \( s \) is a reachable state, and thus add the counterexample to \( S^+(\ell) \).
– Case 4: Invalid heap access inside the loop. The counterexample state is consistent with the candidate loop invariant, but triggers an invalid heap access such as a null access. It is a negative sample and is added to \( S^-(\ell) \).

4.3 Consistency checking

For each prediction returned by the predictor, we check its consistency with the positive and negative samples obtained so far. This is needed because Platypus cannot provide correctness guarantees, and does not make use of negative samples. Thus we check each returned formula \( \varphi_\ell \) for consistency with the observed samples, i.e., \( \forall \hat{H} \in S^+(\ell). \hat{H} \models \varphi_\ell \) and \( \forall \hat{H} \in S^-(\ell). \hat{H} \not\models \varphi_\ell \). As in our sampling strategy, we use the underlying program verifier for this. For this, we translate a state \( \hat{H} \) into a formula \( \varphi_{\hat{H}} \) that describes the sample \( \hat{H} \) exactly, by introducing variables \( n_v \) for each node \( v \) and representing each edge \((n,f,n')\) as \( n.f \rightarrow n' \). Then \( \hat{H} \) is a model of \( \varphi_\ell \) if and only if all models of \( \varphi_{\hat{H}} \) also satisfy \( \varphi_\ell \). However, since by construction \( \varphi_{\hat{H}} \) only has the model \( \hat{H} \), this is equivalent to checking if \( \varphi_{\hat{H}} \land \varphi_\ell \) has a model. This can be checked using a complete program verifier such as GRASShopper by using \( \varphi_{\hat{H}} \land \varphi_\ell \) as precondition of a procedure whose body is \texttt{assert false}.

5 Learning Shape/Data Invariants

Finally, we show how to use samples from program runs to strengthen predicates in memory safety proofs with data invariants. Such shape/data invariants can, for example, be used to prove that a linked list is sorted. We adapted the DOrder procedure [43] originally developed for immutable data in functional programs to our setting, calling our extension DOrderImp. It inherits all relative completeness guarantees of DOrder. Note that while we only discuss linked lists and binary trees here, the procedure is applicable to all linked data structures. The overall analysis Beetle (see Alg. 3) proceeds similarly to our procedure Locust, but takes a memory safety proof as additional input.

DOrder uses a hypothesis domain of atomic predicates used to express shape properties (e.g., list segments) and data properties (e.g., arithmetic relations). We focus on membership properties of heap nodes in a data structure and relations establishing ordering between two nodes found within a data structure.

The main difference of DOrderImp relative to DOrder is the set and semantics of the considered shape predicates. While DOrder can derive these from algebraic type definitions, we extract them from the shape annotations generated by Locust. For a separation logic predicate \( d \), we use \( FP(d) \) to denote the footprint of \( d \), i.e., all nodes in the heap that are part of the data structure described by \( d \). A containment predicate \( u \in FP(d) \) holds if and only if the heap node \( u \) is in the footprint of \( d \). If \( d \) is a list predicate, \( FP(d) : u \rightarrow^+ v \) relates a pair \((u,v)\) to \( d \) if
Algorithm 3: Pseudocode for Beetle

**Input:** Program $P$ and entry procedure $p$ with precondition $\varphi_p$, locations $L$ requiring program annotations, shape annotations $\varphi_{\ell}$ for $\ell \in L$

1. $I \leftarrow$ sample initial states satisfying $\varphi_p$ \{see Sect. 4.1\}
2. $S^+ \leftarrow$ execute $p$ on $I$ to map location $\ell \in L$ to set of observed states
3. **while** true **do**
4.  **for all** $\ell \in L$ **do**
5.  $\varphi_{\ell}^{sd} \leftarrow$ DOrderImp$(\varphi_{\ell}, S^+ (\ell), S^- (\ell))$
6.  $P' \leftarrow$ annotate $P$ with inferred $\varphi_{\ell}^{sd}$
7.  **if** GRASShopper($P'$) returns counterexample $s$ **then**
8.    **if** $s$ is new counterexample **then**
9.      update $S^+, S^-$ to contain $s$ for correct location \{see Sect. 4.2\}
10.  **else** return FAIL
11. **else** return SUCCESS

$u$ occurs before $v$ in $d$ (transitively). Similar definitions are given if $d$ refers to a tree. For example, the predicate $FP(d) : u \prec v$ is satisfied only if $v$ occurs in a subtree of $d$ rooted at $u$. The semantics of ordering predicates directly inherit the semantics of reachability predicates (cf. $\texttt{Btwn}$) in GRASShopper [35].

When inferring shape-data properties at program location $\ell$, we first extract the atomic separation logic predicates (e.g. $\texttt{lseg}(x,y)$) from the given shape annotation $\varphi_{\ell}$ using the function $\texttt{Mem}(\varphi_{\ell})$. We then consider the following set of (well-typed) predicates over the footprints of separation logic predicates in $\varphi_{\ell}$:

$$\Omega_{\text{shape}}(\varphi_{\ell}) = \{ u \in FP(d), FP(d) : u \rightarrow v, FP(d) : u \prec v \mid d \in \text{Mem}(\varphi_{\ell}) \}$$

Our data predicates are binary predicates, which are restricted to range over relational data ordering properties. For this, let $\text{Vars}(\ell)$ be the stack variables in scope at $\ell$ and $u,v$ be two fresh variables not used in the program. Given $\varphi_{\ell}$, the data domain, over some object field $\text{fld}$ containing integer data (denoted by $\Omega_{\text{fld}}$), is constructed from the following atomic predicates

$$\Omega_{\text{fld}}(\ell) = \{ u, \text{fld} \leq x, x \leq u, \text{fld}, u, \text{fld} \leq x, \text{fld}, x, \text{fld} \leq u, \text{fld} \mid x \in \text{Vars}(\ell) \}$$

where only well-typed predicates are considered. While $\Omega_{\text{fld}}$ only permits few predicates, our experiments show that it is sufficient to learn useful properties.

For a given program location $\ell$, we now look for shape/data invariants of the form $\forall u,v.\omega_{\text{shape}} \Rightarrow \psi_{\text{fld}}$ where $\omega_{\text{shape}} \in \Omega_{\text{shape}}(\varphi_{\ell})$ and $\psi_{\text{fld}}$ is an arbitrary boolean combination of predicates from $\Omega_{\text{fld}}(\ell)$. To solve this inference problem, we compute $\forall u,v.\text{Learn}(S^+ (\ell), \Omega_{\text{data}}(\ell), \Omega_{\text{shape}}(\varphi_{\ell}))$ where $\text{Learn}$ implements the relational learning algorithm from $\text{DOrder}$ [43]. In the algorithm, the free variables $u$ and $v$ range over node objects observed in the footprints of the samples in $S^+ (\ell)$. The learned formulas are “separators” between positive and negative samples, such that they are true on all positive samples and false on at least some of the negative samples. This algorithm produces exactly the specifications described in Sect. 2 using our hypothesis domain for the program in Fig. 1. For verification, we translate discovered invariants into annotations and ask GRASShopper to verify them. The translation is straightforward because the ordering predicates follow the reachability predicates in GRASShopper as discussed above.

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6 Experiments & Conclusion

Our tool Cricket combines the procedures Locust and Beetle as an extension of GRASShopper [35] (see Fig. 5 for an overview of all components). Platypus is implemented as a stand-alone tool in F#.

6.1 Experimental Evaluation

We have evaluated our tool on a number of standard example programs. One set are the example programs distributed with GRASShopper that operate on lists with integer data, including standard algorithms such as traversal, filtering, and concatenation of sorted and bounded lists, as well more complex algorithms such as quicksort, mergesort and insertionsort. For these, we prove the “natural” program properties, i.e., that modification of a sorted structure again yields a sorted structure, and that sorting algorithms turn an unsorted list into a sorted list. Furthermore, we considered four simple traversal routines of nested list/tree data structures. We could not obtain another tool that could automatically prove the considered shape/data properties. Instead, we compare Locust as a memory safety prover to S2/HIP [25, 26], Predator [13] and Forester [1]. The full set of results is displayed in Tab. 1, where a ✓ indicates that a tool was successful, and ✗ that it failed (either explicit failure or timeout after 300s). For Platypus, we also note the number of disjuncts in generated invariants, and for Locust and Beetle the number of iterations in the counterexample-refinement loop. As our implementation is not optimized (e.g., each invocation of Platypus starts a new .Net VM and initializes all machine learning components) we do not report runtimes. We cannot distribute our tool at this time due to dependencies on proprietary machine learning components, but have provided detailed log files of the experiments and the examples under https://www.dropbox.com/s/n2trg7naij50yjy/experiment_data.zip and are working on open-sourcing our implementation.

Analysis We find that we can easily prove memory safety of all considered benchmarks. In most cases, Platypus directly predicts the correct shape annotations from the state samples gathered in the initial execution on sampled inputs. Overall, Cricket was able to prove functional correctness of almost all programs (including “hard” cases such as insertionsort with its nested loops and many interacting variables in scope) fully automatically.

Most time spent in Locust is spent on the consistency check of annotations and samples, which could be improved using a more specialized tool. The Cricket failures on double_all and pairwise_sum are due to the fact that the abstract domain used by DOrderImp is insufficient to represent information such as $2 \cdot x = y$. The failure on strand_sort is due to GRASShopper timing out (i.e., needing more than 5 minutes) to check annotations provided by Beetle.
6.2 Conclusion & Future Work

We have presented a new technique for data-driven shape analysis using machine learning techniques, which can be combined with an off-the-shelf program verifier to automatically prove memory safety of heap-manipulating programs. Furthermore, we have combined this with a second technique to strengthen such shape invariants with information about the data contained in the described data structures. All of our contributions have been implemented in our tool Cricket, whose experimental evaluation shows that it is able to automatically prove (functional) correctness of programs that are beyond other state-of-the-art tools.

We plan to extend this work in three aspects. Firstly, we aim to extend Locust to support the introduction of existential quantifiers that Platypus allows. Secondly, one aspect of Platypus that still requires manual and skilled work is feature extraction, which makes it difficult to extend the tool to handle new inductive separation logic predicates precisely. We would like to automate the extraction of relevant features for each production rule, and have already made steps in this direction. We recently introduced Gated Graph Sequence Neural Networks [28] — a technique that leverages deep-learning techniques to make the predictions directly on graph-structured inputs instead of feature vectors. We plan to integrate this into our framework. Initial tests have shown promising results, but some of the features supported by Platypus (most significantly, disjunctive formula predictions) are not yet available in this new method. Finally, we are interested in integrating our method with interactive program verification assistants, to support verification engineers in their daily work.

Acknowledgements We thank Martin Hruška and Quang Loc Le for help with running their tools S2/HIP, Forester, and Predator for the experiments.

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<th>Platypus</th>
<th>Locust</th>
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Table 1: Experimental results of Cricket on example set.
References