# Improving Haskell Theory Exploration

Chris Warburton

*University of Dundee,*
*http://tocai.computing.dundee.ac.uk*

December 7, 2015

**Abstract**

Theory Exploration is a promising approach to improving the quality and understanding of software, above that available through testing, in languages which are amenable to formal analysis such as those based on pure functional programming. Current theory exploration techniques are limited by their use of exponential time algorithms, which we mitigate by intelligently reducing the size of large inputs, using machine learning to preserve the relationships needed for successful exploration.

## 1 Introduction

As computers and software become more sophisticated, and as our reliance on them increases, the importance of *understanding*, *predicting* and *verifying* these systems grows; which is undermined by their ever-increasing complexity. The *functional programming* paradigm has been proposed for addressing these issues [25], in part by constructing programs which are more amenable to mathematical analysis. For example, in pure functional programming all values are *immutable*: defined once and never changed. Hence there is no way for a value to be altered between the point it is introduced and the point it is used, unlike in many *imperative* languages where we may have to search the whole program to ensure the value is not altered by any intermediate code. Similarly, pure functions cannot depend on any state other than their arguments, and hence will always produce repeatable results.

Whilst use of pure functional programming languages, like Haskell and Idris, is relatively rare, their features are well suited to common software engineering practices like *unit testing*; where tasks are broken down into small, easily-specified "units", and tested in isolation for a variety of use-cases. Functional ideas are thus spreading to mainstream software engineering in a more dilute form; seen, for example, in the recent inclusion of first-class functions in Java [27] and C++ [67].

Functional programming is also well suited to less-widespread practices, such as *property checking* (as popularised by QuickCheck) and *theorem proving*, which are promising methods for increasing confidence in software, yet can be prohibitively expensive. Here we investigate how the recent *theory exploration* approach can lower the effort required to pursue these goals, and in particular how machine learning techniques can mitigate the costs of the combinatorial algorithms involved.

Our contributions are:

- A framework for applying theory exploration tools such as QuickSpec to Haskell's existing package system.
- The application of machine learning algorithms to theory exploration, for intelligently discovering interesting sub-sets of large signatures, which are more tractable to explore.
- A novel feature extraction method for transforming Haskell expressions into a form amenable to off-the-shelf learning algorithms.
- A comparison of our methods with existing approaches, both for theory exploration in Haskell, and for machine learning in other languages.

We begin in §2 by providing a formal context for analysing Haskell expressions (§2.1) and the results of theory exploration systems like QuickSpec (§2.3). We give a brief overview of testing approaches and how they relate to Haskell (§2.2), as well as the machine learning approaches we are building on (§2.4.1). We discuss our contributions in more depth in §3, and provide implementation details §4. A variety of related work is surveyed in §5, and we give several potential directions for future research in §7.

# 2 Background

## 2.1 Haskell

We decided to focus on theory exploration in the Haskell programming language as it has mature, state-of-the-art implementations (QuickSpec [12] and HipSpec [11]). This is evident from the fact that the state-of-the-art equivalent for Isabelle/HOL, the Hipster [29] system, is actually implemented by translating to Haskell and invoking HipSpec.

Haskell is well-suited to programming language research; indeed, this was a goal of the language's creators [42]. Like most members of the *functional programming* paradigm, Haskell is essentially a variant of $\lambda$-calculus, with extra features such as a strong type system and "syntactic sugar" to improve readability. For simplicity, we will focus on an intermediate representation of the GHC compiler, known as *GHC Core*, rather than the relatively large and complex syntax of Haskell proper. Core is based on System $F_C$, but for our machine

$$
\begin{array}{rl}
\mathit{expr} & \rightarrow \texttt{Var}\ \mathit{id} \\
 & \mid \texttt{Lit}\ \mathit{literal} \\
 & \mid \texttt{App}\ \mathit{expr}\ \mathit{expr} \\
 & \mid \texttt{Lam}\ \mathcal{L}\ \mathit{expr} \\
 & \mid \texttt{Let}\ \mathit{bind}\ \mathit{expr} \\
 & \mid \texttt{Case}\ \mathit{expr}\ \mathcal{L}\ [\mathit{alt}] \\
 & \mid \texttt{Type} \\
\mathit{id} & \rightarrow \texttt{Local}\ \mathcal{L} \\
 & \mid \texttt{Global}\ \mathcal{G} \\
 & \mid \texttt{Constructor}\ \mathcal{D} \\
\mathit{literal} & \rightarrow \texttt{LitNum}\ \mathcal{N} \\
 & \mid \texttt{LitStr}\ \mathcal{S} \\
\mathit{alt} & \rightarrow \texttt{Alt}\ \mathit{altcon}\ \mathit{expr}\ [\mathcal{L}] \\
\mathit{altcon} & \rightarrow \texttt{DataAlt}\ \mathcal{D} \\
 & \mid \texttt{LitAlt}\ \mathit{literal} \\
 & \mid \texttt{Default} \\
\mathit{bind} & \rightarrow \texttt{NonRec}\ \mathit{binder} \\
 & \mid \texttt{Rec}\ [\mathit{binder}] \\
\mathit{binder} & \rightarrow \texttt{Bind}\ \mathcal{L}\ \mathit{expr}
\end{array}
$$

Where: $\mathcal{S}$ = string literals
$\mathcal{N}$ = numeric literals
$\mathcal{L}$ = local identifiers
$\mathcal{G}$ = global identifiers
$\mathcal{D}$ = constructor identifiers

Figure 1: Simplified syntax of GHC Core in BNF style. [] and ( , ) denote repetition and grouping, respectively.

```
data Nat = Z
         | S Nat

plus :: Nat -> Nat -> Nat
plus    Z  y = y
plus (S x) y = S (plus x y)

mult :: Nat -> Nat -> Nat
mult    Z  y = Z
mult (S x) y = plus y (mult x y)

odd :: Nat -> Bool
odd    Z  = False
odd (S n) = even n

even :: Nat -> Bool
even    Z  = True
even (S n) = odd n
```

Figure 2: A Haskell datatype for Peano numerals with some simple arithmetic functions, including mutually-recursive definitions for `odd` and `even`. `Bool` is Haskell's built in boolean type, which can be regarded as `data Bool = True | False`.

learning purposes we are mostly interested in its syntax; for a more thorough treatment of System $F_C$ and its use in GHC, see [64, Appendix C].

The sub-set of Core we consider is shown in figure 1; compared to the full language [1] our major change is to ignore type hints (such as explicit casts, and differences between types/kinds/coercions). For brevity, we also omit several other forms of literal (machine words of various sizes, individual characters, etc.), as their treatment is similar to those of strings and numerals. We will use quoted strings to denote names and literals, e.g. `Local "foo"`, `Global "bar"`, `Constructor "Baz"`, `LitStr "quux"` and `LitNum "42"`, and require only that they can be compared for equality.

Figure 2 shows some simple Haskell function definitions, along with a custom datatype for Peano numerals. The translation to our Core syntax is routine, and shown in figure 3. Although the Core is more verbose, we can see that similar structure in the Haskell definitions gives rise to similar structure in the Core; for example, the definitions of `odd` and `even` are identical in both languages, except for the global variables. This correspondence allows us to analyse

Note that we exclude representations for type-level entities, including datatype definitions like that of `Nat`. GHC can represent these, but in this work we only consider reducible expressions (i.e. value-level bindings of the form `f a b ...`

[1] As of GHC version 7.10.2, the latest at the time of writing.

plus

```
Lam "a" (Lam "y" (Case (Var (Local "a"))
                       "b"
                       (Alt (DataAlt "Z") (Var (Local "y")))
                       (Alt (DataAlt "S") (App (Var (Constructor "S"))
                                               (App (App (Var (Global "plus"))
                                                         (Var (Local  "x")))
                                                    (Var (Local "y"))))
                                          "x")))
```

mult

```
Lam "a" (Lam "y" (Case (Var (Local "a"))
                       "b"
                       (Alt (DataAlt "Z") (Var (Constructor "Z")))
                       (Alt (DataAlt "S") (App (App (Var (Global "plus"))
                                                    (Var (Local  "y")))
                                               (App (App (Var (Global "mult"))
                                                         (Var (Local  "x")))
                                                    (Var (Local  "y"))))
                                          "x")))
```

odd

```
Lam "a" (Case (Var (Local "a"))
              "b"
              (Alt (DataAlt "Z") (Var (Constructor "False")))
              (Alt (DataAlt "S") (App (Var (Global "even"))
                                      (Var (Local  "n")))
                                 "n"))
```

even

```
Lam "a" (Case (Var (Local "a"))
              "b"
              (Alt (DataAlt "Z") (Var (Constructor "True")))
              (Alt (DataAlt "S") (App (Var (Global "odd"))
                                      (Var (Local  "n")))
                                 "n"))
```

Figure 3: Translations of functions in figure 2 into the Core syntax of figure 1. Notice the introduction of explicit $\lambda$ abstractions (`Lam`) and the use of `Case` to represent piecewise definitions. Fresh variables are chosen arbitrarily as `"a"`, `"b"`, etc.

`= ...`).

## 2.2 QuickCheck

Although unit testing is the de facto industry standard for quality assurance in non-critical systems, the level of confidence it provides is rather low, and totally inadequate for many (e.g. life-) critical systems. To see why, consider the following Haskell function, along with some unit tests:

```
factorial 0 = 1
factorial n = n * factorial (n-1)

fact_base      = factorial 0 == factorial 1
fact_increases = factorial 3 <= factorial 4
fact_div       = factorial 4 == factorial 5 ‘div‘ 5
```

The intent of the function is to map an input $n$ to an output $n!$. The tests check a few properties of the implementation, including the base case, that the function is monotonically increasing, and a relationship between adjacent outputs. However, these tests will *not* expose a serious problem with the implementation: it diverges on half of its possible inputs!

All of Haskell's built-in numeric types allow negative numbers, which this implementation doesn't take into account. Whilst this is a rather trivial example, it highlights a common problem: unit tests are insufficient to expose incorrect assumptions. In this case, our assumption that numbers are positive has caused a bug in the implementation *and* limited the tests we've written.

If we do manage to spot this error, we might capture it in a *regression test* and update the definition of `factorial` to handle negative numbers, e.g. by taking their absolute value:

```
factorial 0 = 1
factorial n = let nPos = abs n
               in nPos * factorial (nPos - 1)

fact_neg = factorial 1 == factorial (-1)
```

However, this is *still* not enough, since this function will also accept fractional values[2], which will also cause it to diverge. Clearly, by choosing what to test we are biasing the test suite towards those cases we've already taken into account, whilst neglecting the problems we did not expect.

Haskell offers a partial solution to this problem in the form of *property checking*. Tools such as QuickCheck separate tests into three components: a *property* to check, which unlike a unit test may contain *free variables*; a source of values to instantiate these free variables; and a stopping criterion. Here is how we might restate our unit tests as properties:

[2] Since we only use generic numeric operations, the function will be polymorphic with a type of the form `forall t. Num t => t -> t`, where `Num t` constrains the type variable `t` to be numeric. In fact, Haskell will infer extra constraints such as `Eq t` since we have used `==` in the unit tests.

```
fact_base        = factorial 0 == factorial 1
fact_increases n = factorial n <= factorial (n+1)
fact_div       n = factorial n == factorial (n+1) ‘div‘ (n+1)
fact_neg       n = factorial n == factorial (-n)
```

The free variables (all called `n` in this case) are abstracted as function parameters; these parameters are implicitly *universally quantified*, i.e. we've gone from a unit test asserting $factorial(3) \leq factorial(4)$ to a property asserting $\forall n, factorial(n) \leq factorial(n+1)$. Notice that unit tests like `fact_base` are valid properties; they just assert rather weak statements.

To check these properties, QuickCheck treats closed terms (like `fact_base`) just like unit tests: pass if they evaluate to `True`, fail otherwise. For open terms, a random selection of values are generated and passed in via the function parameter; the results are then treated in the same way as closed terms. The default stopping criterion for QuickCheck (for each test) is when a single generated test fails, or when 100 generated tests pass.

The ability to state *universal* properties in this way avoids some of the bias we encountered with unit tests. In the `factorial` example, this manifests in two ways:

- QuickCheck cannot test polymorphic functions; they must be *monomorphised* first (instantiated to a particular concrete type). This is a technical limitation, since QuickCheck must know which type of values to generate, but in our example it would bring the issue with fractional values to our attention.

- The generators used by QuickCheck depend only on the *type* of value they are generating: since `Int` includes positive and negative values, the `Int` generator will output both. This will expose the problem with negative numbers, which we weren't expecting.

Property checking is certainly an improvement over unit testing, but the problem of tests being biased towards expected cases remains, since we are manually specifying the properties to be checked.

We can reduce this bias further through the use of *theory exploration* tools, such as QuickSpec and HipSpec. These programs *discover* properties of a "theory" (e.g. a library), through a combination of brute-force enumeration, random testing and (in the case of HipSpec) automated theorem proving.

## 2.3 Theory Exploration

In this work we consider the problem of *(automated) theory exploration*, which includes the ability to *generate* conjectures about code, to *prove* those conjectures, and hence output *novel* theorems without guidance from the user. The method of conjecture generation is a key characteristic of any theory exploration system, although all existing implementations rely on brute force enumeration to some degree.

We focus on QuickSpec [12], which conjectures equations about Haskell code (these may be fed into another tool, such as HipSpec, for proving). These conjectures are arrived at through the following stages:

1. Given a typed signature $\Sigma$ and set of variables $V$, QuickSpec generates a list *terms* containing the functions and constants from $\Sigma$, the variables from $V$ and type-correct function applications $f(x)$, where $f$ and $x$ are elements of *terms*. To ensure the list is finite, function applications are only nested up to a specified depth (by default, 3).
2. The elements of *terms* are grouped into equivalence classes, based on their type.
3. Each variable is instantiated to a particular value, generated randomly by QuickCheck.
4. For each class, the members are compared (using a pre-specified function, such as equality `==`) to see if these instantiations have caused an observable difference between members. If so, the class is split up to separate such distinguishable members.
5. The previous steps of variable instantiation and comparison are repeated until the classes stabilise (i.e. no differences have been observed for some specified number of repetitions).
6. A set of equations are then conjectured, relating each class's members.

Such *conjectures* can be used in several ways: they can be simplified for direct presentation to the user (by removing any equation which can be derived from the others by rewriting), sent to a more rigorous system like HipSpec or Hipster for proving, or even serve as a background theory for an automated theorem prover [11].

As an example, we can consider a simple signature containing the expressions from figure 2:

$$\Sigma_{\texttt{Nat}} = \{\texttt{Z}, \texttt{S}, \texttt{plus}, \texttt{mult}, \texttt{odd}, \texttt{even}\}$$

Together with a set of variables, say $V_{\texttt{Nat}} = \{a, b, c\}$, QuickSpec's enumeration will resemble the following:

$$\begin{aligned} terms_{\texttt{Nat}} = [&\texttt{Z},\ \texttt{S},\ \texttt{plus},\ \texttt{mult},\ \texttt{odd},\ \texttt{even},\ a,\ b,\ c,\ \texttt{S Z},\ \texttt{S}\ a,\ \texttt{S}\ b,\\ &\texttt{S}\ c,\ \texttt{plus Z},\ \texttt{plus}\ a,\ \dots] \end{aligned}$$

Notice that Haskell curries functions, so the binary functions `plus` and `mult` can be treated as unary functions which return unary functions. This is required as the construction of *terms* applies functions to one argument at a time.

```
                  plus a b = plus b a
                  plus a Z = a
         plus a (plus b c) = plus b (plus a c)
                  mult a b = mult b a
                  mult a Z = Z
         mult a (mult b c) = mult b (mult a c)
              plus a (S b) = S (plus a b)
              mult a (S b) = plus a (mult a b)
         mult a (plus b b) = mult b (plus a a)
                 odd (S a) = even a
            odd (plus a a) = odd Z
           odd (times a a) = odd a
                even (S a) = odd a
           even (plus a a) = even Z
          even (times a a) = even a
plus (mult a b) (mult a c) = mult a (plus b c)
```

Figure 4: Equations conjectured by QuickSpec for the functions in figure 2; after simplification.

These terms will be grouped into five classes, one each for `Nat`, `Nat -> Nat`, `Nat -> Nat -> Nat`, `Nat -> Bool` and `Bool`. As the variables $a$, $b$ and $c$ are instantiated to various randomly-generated numbers, these equivalence classes will be divided, until eventually the equations in figure 4 are conjectured.

Although complete, this enumeration approach is wasteful: many terms are unlikely to appear in theorems, which requires careful choice by the user of what to include in the signature. Here we know that addition and multiplication are closely related, and hence obey many algebraic laws. Our machine learning technique aims to predict these kinds of relations between functions, so we can create small signatures which nevertheless have the potential to give rise to many equations.

QuickSpec (and HipSpec) is also compatible with Haskell's existing testing infrastructure, such that an invocation of `cabal test` can run these tools alongside more traditional QA tools like QuickCheck, HUnit and Criterion.

In fact, there are similarities between the way a TE system like QuickSpec can generalise from checking *particular* properties to *inventing* new ones, and the way counterexample finders like QuickCheck can generalise from testing *particular* expressions to *inventing* expressions to test. One of our aims is to understand the implications of this generalisation, the lessons that each can learn from the other's approach to term generation, and the consequences for testing and QA in general.

## 2.4 Clustering

Our approach to scaling up QuickSpec takes inspiration from two sources. The first is premise selection, which makes expensive algorithms used in theorem proving more practical by limiting the size of their inputs. We describe this approach in more details in §5.2. Premise selection is a practical tool which has existing applications in software, such as the *Sledgehammer* component of the Isabelle/HOL theorem prover.

Despite the idea's promise, we cannot simply invoke existing premise selection algorithms in our theory exploration setting. The reason is that premise selection requires a distinguished expression to compare everything against; in practice this is the current goal of a theorem prover. Theory exploration does not have such a distinguished expression; instead, we are interested in relationships between *any* terms generated from a signature, and hence we must consider the relevance of *all terms* to *all other terms*.

A natural fit for this task is *clustering*, which attempts to group similar inputs together in an unsupervised way. Based on their success in discovering relationships and patterns between expressions in Coq and ACL2 (in the ML4PG and ACL2(ml) tools respectively), we hypothesise that clustering methods can fulfil the role of relevance filters for theory exploration: intelligently breaking up large signatures into smaller ones more amenable to brute force enumeration, such that related expressions are explored together.

### 2.4.1 Feature Extraction

Before describing clustering in detail, we must introduce the idea of *feature extraction*. This is the conversion of "raw" input data, such as audio, images or (in our case) Core expressions, into a form more suited to machine learning algorithms. By pre-processing our data in this way, we can re-use the same "off-the-shelf" machine learning algorithms in a variety of domains.

We use a standard representation of features as a *feature vector* of numbers $(x_1, \dots, x_d)$ where $x_i \in \mathbb{R}$. [3] For learning purposes this has some important advantages over raw expressions:

Another benefit of feature extraction is to *normalise* the input data to a fixed-size representation.

- All of our feature vectors will be the same size, i.e. they will all have length (or *dimension*) $d$. Many ML algorithms only work with inputs of a uniform size; feature extraction allows us to use these algorithms in domains where the size of each input is not known, may vary or may even be unbounded. For example, element-wise comparison of feature vectors is trivial (compare the $i$th elements for $1 \leq i \leq d$); for expressions this is not so straightforward, as their nesting may give rise to very different shapes.

[3] In fact, ractical implementations will use an approximate format such as IEEE 754 floating point numbers.

- Unlike our expressions, which are discrete, we can continuously transform one feature vector into another. This enables many powerful ML algorithms to be used, such as those based on *gradient descent* or, in our case, arithmetic means.

- Feature vectors can be chosen to represent the relevant information in a more compressed form than the raw data; for example, we might replace verbose, descriptive identifiers with sequential numbers. This reduces the input size of the machine learning problem, improving efficiency.

### 2.4.2 k-Means

Clustering is an unsupervised machine learning task for grouping $n$ data points using a similarity metric. There are many variations on this theme, but in our case we make the following choices:

- We fix the number of clusters at $k = \lceil \sqrt{n} \rceil$.

- Data points will be $d$-dimensional feature vectors, as defined above.

- We will use euclidean distance (denoted $e$) as our similarity metric.

- We will use *k-means* clustering, implemented by Lloyd's algorithm.

This is a standard setup, supported by off-the-shelf tools. In particular, it is similar to that used by the ML4PG and ACL2(ml), which makes our results more easily comparable.

k-means works, as the name suggests, by calculating the *mean value* of each cluster, which we define as:

$$\overline{X}_i = \frac{\sum_{x \in X} x_i}{|X|}$$

Since k-means is iterative, we will use function notation to denote time steps, so $x(t)$ denotes the value of $x$ at time $t$. We denote the clusters as $C^1$ to $C^k$ and their mean values as $\mathbf{m}^1$ to $\mathbf{m}^k$, hence:

$$\mathbf{m}^i(t) = \overline{C}^i(t) \quad \text{for } t > 0$$

Before k-means starts, we must choose *seed* values for $\mathbf{m}^i(0)$. Many methods have been proposed for choosing these values [3]. For simplicity, we will choose values randomly from our data set $S$; this is known as the Forgy method.

The elements of each cluster $C^i(t)$ are those data points closest to the mean value at the previous time step:

$$C^i(t) = \{\mathbf{x} \in S \mid i = \operatorname*{argmin}_j e(\mathbf{x}, \mathbf{m}^j(t-1))\} \quad \text{for } t > 0$$

As $t$ increases, the clusters $C^i$ move from their initial location around the "seeds", to converge on a local minimum of the "within-cluster sum of squared error" objective:

$$\underset{C}{\operatorname{argmin}} \sum_{i=1}^{k} \sum_{\mathbf{x} \in C^i} e(\mathbf{x}, \mathbf{m}^i)^2$$

# 3 Contributions

## 3.1 Recurrent Clustering

We take the *recurrent clustering* approach found in ML4PG and ACL2(ml), and implement a variant in the context of Haskell theory exploration. As a clustering algorithm, the aim of recurrent clustering is to identify similarities in a set of data points (in our case, Core expressions). Its distinguishing characteristic is to *combine* feature extraction and clustering into a single recursive algorithm (shown as algorithm 1), which goes beyond a simple syntactic characterisation, to allow the features of an expression to depend on those it references. Here we describe our approach to recurrent clustering and compare its similarity and differences to those of ML4PG and ACL2(ml).

We consider our algorithm in two stages: the first transforms the nested structure of expressions into a flat feature vector representation; the second converts the discrete symbols of Core syntax into features (real numbers), which we will denote using the notation $\ulcorner\urcorner$.

### 3.1.1 Expressions to Vectors

Our recurrent clustering algorithm makes use of the k-means algorithm described in §2.4.2, which considers the elements of a feature vector to be *orthogonal*. Hence we must ensure that similar expressions not only give rise to similar numerical values, but crucially that these values appear *at the same position* in the feature vectors. Since different patterns of nesting can alter the "shape" of expressions, simple traversals (breadth-first, depth-first, post-order, etc.) may cause features from equivalent sub-expressions to be mis-aligned. For example, consider the following expressions, which represent pattern-match clauses with different patterns but the same body (`Var (Local "y")`):

$$\begin{aligned} X &= \texttt{Alt}\ (\texttt{DataAlt "C"})\ (\texttt{Var}\ (\texttt{Local "y"})) \\ Y &= \texttt{Alt}\ \texttt{Default}\ \qquad\quad (\texttt{Var}\ (\texttt{Local "y"})) \end{aligned}$$

If we traverse these expressions in breadth-first order, converting each token to a feature using $\ulcorner\urcorner$ and padding to the same length with 0, we would get the following feature vectors:

$$\begin{aligned} \mathit{breadthFirst}(X) &= (\ulcorner\texttt{Alt}\urcorner, \ulcorner\texttt{DataAlt}\urcorner, \ulcorner\texttt{Var}\urcorner, \ulcorner\texttt{"C"}\urcorner, \quad \ulcorner\texttt{Local}\urcorner, \ulcorner\texttt{"y"}\urcorner) \\ \mathit{breadthFirst}(Y) &= (\ulcorner\texttt{Alt}\urcorner, \ulcorner\texttt{Default}\urcorner, \ulcorner\texttt{Var}\urcorner, \ulcorner\texttt{Local}\urcorner, \ulcorner\texttt{"y"}\urcorner, \quad 0 \quad\ ) \end{aligned}$$

Here the features corresponding to the common sub-expression `Local "y"` are misaligned, such that only $\frac{1}{3}$ of features are guaranteed to match (others may match by coincidence, depending on $\ulcorner\urcorner$). These feature vectors might be deemed very dissimilar during clustering, despite the intuitive similarity of the expressions $X$ and $Y$ from which they derive.

If we were to align these feature optimally, by padding the fourth column rather than the sixth, then $\frac{2}{3}$ of features would be guaranteed to match, making the similarity of the vectors more closely match our intuition and depend less on coincidence.

The method we use to "flatten" expressions, described below, is a variation of breadth-first traversal which pads each level of nesting to a fixed size $c$ (for *columns*). This doesn't guarantee alignment, but it does prevent mis-alignment from accumulating across different levels of nesting. Our method would align these features into the following vectors, if $c = 2$: [4]

$$\begin{aligned} featureVec(X) &= (\ulcorner\texttt{Alt}\urcorner, 0, \ulcorner\texttt{DataAlt}\urcorner, \ulcorner\texttt{Var}\urcorner, \ulcorner\texttt{"C"}\urcorner, \ulcorner\texttt{Local}\urcorner, \ulcorner\texttt{"y"}\urcorner, 0)\\ featureVec(Y) &= (\ulcorner\texttt{Alt}\urcorner, 0, \ulcorner\texttt{Default}\urcorner, \ulcorner\texttt{Var}\urcorner, \ulcorner\texttt{Local}\urcorner, 0, \ulcorner\texttt{"y"}\urcorner, 0)\end{aligned}$$

Here $\frac{1}{2}$ of the original 6 features align, which is more than $breadthFirst$ but not optimal. Both vectors have also been padded by an extra 2 zeros compared to $breadthFirst$; raising their alignment to $\frac{5}{8}$.

To perform this flattening we first transform the nested tokens of an expression into a *rose tree* of features, using the $toTree$ function shown in figure 5. Rose trees are defined recursively: $T$ is a rose tree if $T = (f, T_1, \dots, T_{n_T})$, where $f \in \mathbb{R}$ and $T_i$ are rose trees. $T_i$ are the *sub-trees* of $T$ and $f$ is the *feature at* $T$. $n_T$ may differ for each (sub-) tree; trees where $n_T = 0$ are *leaves*. The results are illustrated in figure 6a.

These rose trees are then turned into matrices, as shown in figure 6b, by gathering the features of adjacent (sub-) trees at each level of nesting, and concatenating them together (written as $+\!\!+$ ):

$$level(l, (f, T_1, \dots, T_{n_T})) = \begin{cases} (f) & \text{if } l = 1 \\ level(l-1, T_1) +\!\!+ \dots +\!\!+ level(l-1, T_{n_T}) & \text{if } l > 1 \end{cases}$$

Given a rose tree $t$ we can define its matrix $\mathbf{M}$ by $\mathbf{M}_i = pad(level(i, t))$, where $pad$ either truncates or appends zeros, until the row has a fixed length $c$. We also truncate/pad the number of rows to match a fixed number $r$. This way, all expressions give rise to $r \times c$ matrices, where the left-most features at each each level are aligned.

Feature vectors are then simply the concatenation of matrix rows $\mathbf{M}_{1,1} +\!\!+ \mathbf{M}_{1,2} +\!\!+ \dots +\!\!+ \mathbf{M}_{2,1} +\!\!+ \mathbf{M}_{2,2} +\!\!+ \dots$, as shown in figure 6c:

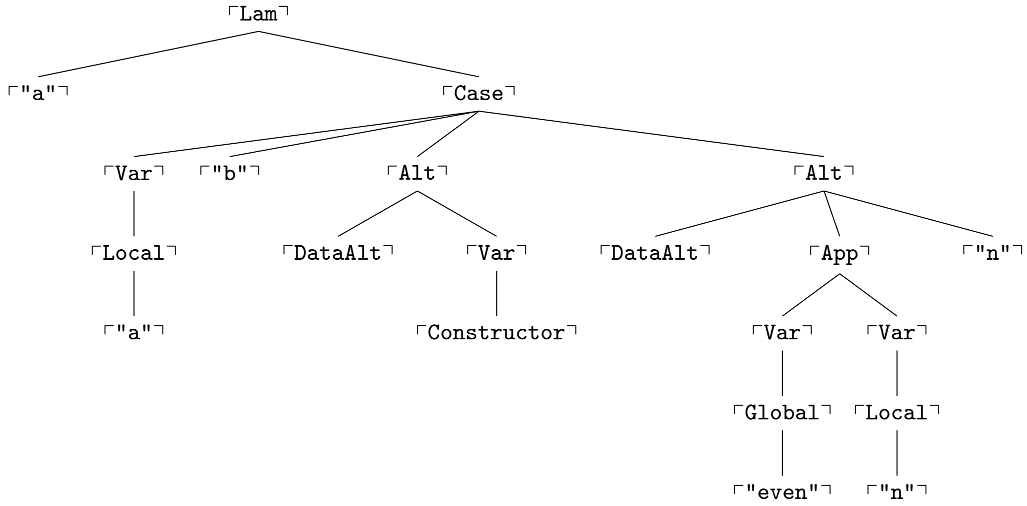
$$featureVec(e) = pad(level(1, toTree(e))) +\!\!+ \dots +\!\!+ pad(level(r, toTree(e))) \tag{1}$$

[4] In fact, the $toTree$ function would ignore the constructor identifier `"C"` and never produce the feature $\ulcorner\texttt{"C"}\urcorner$. However, this example is still accurate in terms of laying out the features as given.

$$
toTree(e) = \begin{cases}
(\ulcorner\texttt{Var}\urcorner, toTree(e_1)) & \text{if } e = \texttt{Var}\ e_1 \\
(\ulcorner\texttt{Lit}\urcorner, toTree(e_1)) & \text{if } e = \texttt{Lit}\ e_1 \\
(\ulcorner\texttt{App}\urcorner, toTree(e_1), toTree(e_2)) & \text{if } e = \texttt{App}\ e_1\ e_2 \\
(\ulcorner\texttt{Lam}\urcorner, toTree(e_1)) & \text{if } e = \texttt{Lam}\ l_1\ e_1 \\
(\ulcorner\texttt{Let}\urcorner, toTree(e_1), toTree(e_2)) & \text{if } e = \texttt{Let}\ e_1\ e_2 \\
(\ulcorner\texttt{Case}\urcorner, toTree(e_1), toTree(a_1), \dots) & \text{if } e = \texttt{Case}\ e_1\ l_1 a_1 \dots \\
(\ulcorner\texttt{Type}\urcorner) & \text{if } e = \texttt{Type} \\
(\ulcorner\texttt{Local}\urcorner, leaf(l_1)) & \text{if } e = \texttt{Local}\ l_1 \\
(\ulcorner\texttt{Global}\urcorner, leaf(g_1)) & \text{if } e = \texttt{Global}\ g_1 \\
(\ulcorner\texttt{Constructor}\urcorner) & \text{if } e = \texttt{Constructor}\ d_1 \\
(\ulcorner\texttt{LitNum}\urcorner) & \text{if } e = \texttt{LitNum}\ n_1 \\
(\ulcorner\texttt{LitStr}\urcorner) & \text{if } e = \texttt{LitStr}\ s_1 \\
(\ulcorner\texttt{Alt}\urcorner, toTree(e_1), toTree(e_2)) & \text{if } e = \texttt{Alt}\ e_1 e_2 l_1 \dots \\
(\ulcorner\texttt{DataAlt}\urcorner) & \text{if } e = \texttt{DataAlt}\ g_1 \\
(\ulcorner\texttt{LitAlt}\urcorner, toTree(e_1)) & \text{if } e = \texttt{LitAlt}\ e_1 \\
(\ulcorner\texttt{Default}\urcorner) & \text{if } e = \texttt{Default} \\
(\ulcorner\texttt{NonRec}\urcorner, toTree(e_1)) & \text{if } e = \texttt{NonRec}\ e_1 \\
(\ulcorner\texttt{Rec}\urcorner, toTree(e_1), \dots) & \text{if } e = \texttt{Rec}\ e_1 \dots \\
(\ulcorner\texttt{Bind}\urcorner, toTree(e_1)) & \text{if } e = \texttt{Bind}\ l_1 e_1
\end{cases}
$$

$$
leaf(x) = (\ulcorner x \urcorner)
$$

Figure 5: Transforming Core expressions of figure 1 to rose trees. The recursive definition is mostly routine; each repeated element (shown as $\dots$) has an example to indicate their handling, e.g. for `Rec` we apply $toTree$ to each $e_i$. We ignore values of $\mathcal{D}$ as constructors can only be distinguished by their type, which we do not currently support. We also ignore values from $\mathcal{S}$ and $\mathcal{N}$ as it simplifies our later definition of $\ulcorner\urcorner$, and we conjecture that the effect on clustering real code is low.



(a) Rose tree for the expression `odd` from figure 3. Each (sub-) rose tree is rendered with its feature at the node and sub-trees beneath.

$$\begin{bmatrix}
\ulcorner\texttt{Lam}\urcorner & 0 & 0 & 0 & 0 & 0 \\
\ulcorner\texttt{"a"}\urcorner & \ulcorner\texttt{Case}\urcorner & 0 & 0 & 0 & 0 \\
\ulcorner\texttt{Var}\urcorner & \ulcorner\texttt{"b"}\urcorner & \ulcorner\texttt{Alt}\urcorner & \ulcorner\texttt{Alt}\urcorner & 0 & 0 \\
\ulcorner\texttt{Local}\urcorner & \ulcorner\texttt{DataAlt}\urcorner & \ulcorner\texttt{Var}\urcorner & \ulcorner\texttt{DataAlt}\urcorner & \ulcorner\texttt{App}\urcorner & \ulcorner\texttt{"n"}\urcorner \\
\ulcorner\texttt{"a"}\urcorner & \ulcorner\texttt{Constructor}\urcorner & \ulcorner\texttt{Var}\urcorner & \ulcorner\texttt{Var}\urcorner & 0 & 0 \\
\ulcorner\texttt{Global}\urcorner & \ulcorner\texttt{Local}\urcorner & 0 & 0 & 0 & 0 \\
\ulcorner\texttt{"even"}\urcorner & \ulcorner\texttt{"n"}\urcorner & 0 & 0 & 0 & 0
\end{bmatrix}$$

(b) Matrix generated from figure 6a, padded to 6 columns. Each level of nesting in the tree corresponds to a row in the matrix.

$$(\ulcorner\texttt{Lam}\urcorner, 0, 0, 0, 0, 0, \ulcorner\texttt{"a"}\urcorner, \ulcorner\texttt{Case}\urcorner, 0, 0, 0, 0, \ulcorner\texttt{Var}\urcorner, \ulcorner\texttt{"b"}\urcorner, \ulcorner\texttt{Alt}\urcorner, \ulcorner\texttt{Alt}\urcorner, 0, 0, \ldots$$

(c) (Prefix of) the feature vector for `odd`, constructed by concatenating the rows of 6b. Ignoring padding, the features are in breadth-first order.

Figure 6: Feature extraction applied to the expression `odd` from figure 3.

### 3.1.2 Symbols to Features

We now define the algorithm for $\ulcorner\urcorner$, which turns terminal symbols of Core syntax into features (real numbers). For known language features, such as $\ulcorner\texttt{Lam}\urcorner$ and $\ulcorner\texttt{Case}\urcorner$, we can enumerate the possibilities and assign a value to each, in a similar way to [21] in Coq. We use a constant $\alpha$ to separate these values from those of other tokens (e.g. identifiers), but the order is essentially arbitrary: [5]

$$\begin{array}{rrr}
\ulcorner\texttt{Alt}\urcorner = \alpha & \ulcorner\texttt{DataAlt}\urcorner = \alpha + 1 & \ulcorner\texttt{LitAlt}\urcorner = \alpha + 2 \\
\ulcorner\texttt{Default}\urcorner = \alpha + 3 & \ulcorner\texttt{NonRec}\urcorner = \alpha + 4 & \ulcorner\texttt{Rec}\urcorner = \alpha + 5 \\
\ulcorner\texttt{Bind}\urcorner = \alpha + 6 & \ulcorner\texttt{Let}\urcorner = \alpha + 7 & \ulcorner\texttt{Case}\urcorner = \alpha + 8 \\
\ulcorner\texttt{Local}\urcorner = \alpha + 9 & \ulcorner\texttt{Global}\urcorner = \alpha + 10 & \ulcorner\texttt{Constructor}\urcorner = \alpha + 11 \\
\ulcorner\texttt{Var}\urcorner = \alpha + 12 & \ulcorner\texttt{Lam}\urcorner = \alpha + 13 & \ulcorner\texttt{App}\urcorner = \alpha + 14 \\
\ulcorner\texttt{Type}\urcorner = \alpha + 15 & \ulcorner\texttt{Lit}\urcorner = \alpha + 16 & \ulcorner\texttt{LitNum}\urcorner = \alpha + 17 \\
\ulcorner\texttt{LitStr}\urcorner = \alpha + 18 & &
\end{array}$$

To encode *local* identifiers $\mathcal{L}$ we use their *de Bruijn index*, since this is a numeric value suitable for use as a feature, and it gives equal values for $\alpha$-equivalent expressions. To calculate these indices the *toTree* function maintains a *context* as it recurses through expressions (we elided this from figure 5 for clarity). The context is a list of the local identifiers which are in scope, prepended as they are encountered. The context is initially empty, and only extended when *toTree* calls itself recursively.

For example, when calculating $\mathit{toTree}(\texttt{Lam}\ i\ e)$ in context $x$, we make the recursive call $\mathit{toTree}(e)$ in the context of $x$ *prepended with* $i$ (i.e. $(i) +\!\!+\, x$). Similar extensions of the context are performed in the cases of `Bind`, `Case`[6], `Alt` (which may introduce an arbitrary number of local identifiers) and `Let` (where identifiers are taken from occurrences of `Bind` in the first expression).

Well-formed Haskell declarations do not contain free variables (or, equivalently, free variables are encoded as global identifiers rather than local identifiers). Hence if we apply *toTree* to (the Core expression corresponding to) such declarations we are guaranteed that $l \in \mathcal{L}$ will appear in the context whenever we encounter $\ulcorner l\urcorner$. In which case we define:

$$\ulcorner l\urcorner = i + 2\alpha \quad \text{if } l \in \mathcal{L} \tag{2}$$

Where $i$ is the index of the first occurrence of $l$ in the context; this is the de Bruijn index of $l$. We again use $\alpha$ to separate these features from those of other constructs.

[5] In [21], "similar" Gallina tokens like `fix` and `cofix` are grouped together to reduce redundancy; we do not group tokens, but we do put "similar" tokens close together, such as `Local` and `Global`.

[6] The $\mathcal{L}$ value in a `Case` expression is bound to the expression being matched against; a technical detail to preserve sharing.

Since the *toTree* function discards numerals, strings and constructor identifiers, the only remaining case is global identifiers $\mathcal{G}$. Since these are declared *outside* the body of an expression, we cannot perform the same indexing trick as we did for local identifiers. We also cannot directly encode the form of the identifiers, e.g. using a scheme like Gödel numbering, since this is essentially arbitrary and has no effect on their semantic meaning (referencing other expressions).

Instead, we encode global identifiers *indirectly*, by looking up the expressions which they *reference*. For $g \in \mathcal{G}$ we define $\ulcorner g \urcorner$ as the *index of the cluster which* $g$ *appears in*. This is where the recurrent nature of the algorithm appears, since we perform k-means clustering *during* feature extraction, and that clustering step, in turn, requires that we perform feature extraction.

For this recursive process to be well-founded, we impose a topological ordering on declarations based on their dependencies (the expressions they reference). This is slightly complicated in Haskell (compared to Coq, for example), since general recursion is permitted and hence the dependency graph may contain cycles. To handle this, we perform the sort using an algorithm such as Tarjan's which produces a sorted list of *strongly connected components* (SCCs), where each SCC is a mutually-recursive sub-set of the declarations. References which point to the same SCC as the expression they appear in (which includes direct recursion and mutual recursion) are given a constant feature value $f_{recursion}$.

By working through the sorted list of SCCs, storing the features of each top-level expression as they are calculated, our algorithm can be computed *iteratively* rather than recursively, as shown in algorithm 1. This makes cyclic references particularly easy to handle: global identifiers are looked up in the current clusters $C$, and if not found the value $f_{recursion}$ is used.

**Algorithm 1** Recurrent clustering of Core expressions.

```
Require: List $d$ contains SCCs of (identifier, expression) pairs, in dependency order.
procedure RecurrentCluster
    $C \leftarrow []$
    $DB \leftarrow \varnothing$
    for all $scc$ in $d$ do
        $DB \leftarrow DB \cup \{(i, featureVec(e)) \mid (i, e) \in scc\}$
        $C \leftarrow kMeans(DB)$
    return $C$
```

As an example of this recurrent process, we can consider the Peano arithmetic functions from figure 3. A valid topological ordering would be (eliding Core expressions to save space) $d = [\{(\texttt{plus}, \dots)\}, \{(\texttt{odd}, \dots), (\texttt{even}, \dots)\}, \{(\texttt{mult}, \dots)\}]$:

- The first iteration through RecurrentCluster's loop will set $scc \leftarrow \{(\texttt{plus}, \dots)\}$.
- With $i = \texttt{plus}$ and $e$ as its Core expression, calculating $featureVec(e)$

is straightforward; the recursive call $\ulcorner$`plus`$\urcorner$ will become $f_{recursion}$ (since `plus` doesn't appear in $C$).

- The call to *kMeans* will produce $C \leftarrow [\{\texttt{plus}\}]$, i.e. a single cluster containing `plus`.
- The next iteration will set $scc \leftarrow \{(\texttt{odd}, \dots), (\texttt{even}, \dots)\}$.
- With $i = \texttt{odd}$ and $e$ as its Core expression, the call to `even` will result in $f_{recursion}$.
- Likewise for the call to `even` when $i = \texttt{odd}$.
- Since the feature vectors for `odd` and `even` will be identical, *kMeans* will put them in the same cluster. The number of clusters $k = \lceil \sqrt{|DB|} \rceil = 2$, so the other cluster must contain `plus`. Their order is arbitrary, so one possibility is $C = [\{\texttt{odd}, \texttt{even}\}, \{\texttt{plus}\}]$.
- Finally `mult` will be clustered. The recursive call will become $f_{recursion}$ whilst the call to `plus` will become 2, since $\texttt{plus} \in C_2$.
- Since $k = 2$, the resulting clusters will be $C \leftarrow [\{\texttt{odd}, \texttt{even}\}, \{\texttt{plus}, \texttt{mult}\}]$.

Even in this very simple example we can see a few features of our algorithm emerge. For example, `odd` and `even` will always appear in the same cluster, since they only differ in their choice of constructor names (which are discarded by *toTree*) and recursive calls (which are replaced by $f_{recursion}$). A more extensive investigation of these features requires a concrete implementation, in particular to pin down values for the parameters such as $r$, $c$, $f_{recursion}$, $\alpha$ and so on.

### 3.1.3 Comparison

Our algorithm is most similar to that of ML4PG, as our transformation maps the elements of a syntax tree to distinct cells in a matrix. In contrast, the matrices produced by ACL2(ml) *summarise* the tree elements: providing, for each level of the tree, the number of variables, nullary symbols, unary symbols, etc.

There are two major differences between our algorithm and that of ML4PG: mutual-recursion and types.

The special handling required for mutual recursion is discussed above (namely, topological sorting of expressions and the $f_{recursion}$ feature). Such handling is not present in ML4PG, since the Coq code it analyses must, by virtue of the language, be written in dependency order to begin with. Coq *does* have limited support for mutually-recursive functions, of the following form:

```
Fixpoint even n := match n with
                      | O   => true
                      | S m => odd m
                   end
    with odd  n := match n with
                      | O   => false
                      | S m => even m
                   end.
```

However, this is relatively uncommon and unsupported by ML4PG.

The more interesting differences come from our handling (or lack thereof) for types. Coq and ACL2 are at opposite ends of the typing spectrum, with the former treating types as first class entities of the language whilst the latter is untyped (or *unityped*). In both cases, we have a *single* language to analyse, by ML4PG and ACL2(ml) respectively.[7]

The situation is different for Haskell, where the type level is distinct from the value level, and there are strict rules for how they can influence each other. In particular, Haskell values can depend on types (via the type class mechanism) but types cannot depend on values.

In our initial approach, we restrict ourselves to the value level. This has several consequences:

- Although they are values, we cannot distinguish between data constructors, other than using exact equality. Hence they are discarded by *toTree*.
- Since Core uses a single `Lam` abstraction for both value- and type-level parameters, we cannot always distinguish between them. This can cause a function's Core arity to be greater than its Haskell arity.

There is certainly promise in including types in our analysis, by pairing every term with its type as in ML4PG. This will allow fine-grained distinction of expressions which are otherwise identical, especially data constructors. Integrating types into our algorithm, and extracting them from Core expressions, is hence left as future work.

# 4 Implementation

We have implemented these ideas in a theory exploration framework called ML4HS. It contains several components.

## 4.1 Recurrent Clustering

Our implementation is a rather direct translation of the algorithm described in §3 into Haskell. At the top level, we send named expressions to `recurrentCluster`, topologically sorted: if an element contains multiple `(Global, Expr)` pairs, they are mutually-recursive:

```
recurrentCluster :: [[(Global, Expr)]] -> [[Global]]
recurrentCluster = go ([],[])
  where go (fs, db) []       = db
```

[7] ML4PG can also analyse Coq's Ltac meta-language. Haskell has its own meta-language, Template Haskell, but here we only consider the regular Haskell which it generates.

```
        go (fs, db) (es:ess) = let fs' = fs ++ map (extract db) es
                                   db' = kMeans fs'
                                in go (fs', db') ess
        extract db (i, e) = (i, rt db e)
```

The overall result of the recurrentCluster function is a list of clusters, containing the IDs of their elements. These are obtained by interleaving clustering (the kMeans function) and feature extraction (the rt function).

The feature extraction itself contains two parts: first, syntax trees matching the grammar in figure 1 are converted into RoseTrees with features (Floats) on their Nodes:

```
data RoseTree = Node Feature [RoseTree]

eRT :: [Local] -> [[Global]] -> Expr -> RoseTree
eRT env db e = case e of
  ...
```

The easiest branches to handle are literals and types, which we represent using particular feature values (sLITNUM, sLITSTR and sTYPE):

```
Lit (LitNum _) -> Node sLITNUM []
Lit (LitStr _) -> Node sLITSTR []
Type           -> Node sTYPE   []
```

Function application simply recurses into both sub-expressions:

```
App e1 e2 -> Node sAPP [eRT env db e1,
                        eRT env db e2]
```

To look up variables locally and globally, we use the lookupL and lookupG functions, respectively. These return the index containing their argument, if found. In the case of lookupL, this acts as a de Bruijn index to give alpha-equivalent terms equal feature vectors. For lookupG, this is the ID of the cluster it appears in; this ensures that references to similar expressions result in similar features:

```
Var (Global i) -> Node (lookupG db  i) []
Var (Local  i) -> Node (lookupL env i) []
```

Finally, when we traverse binders we must extend the environment env:

```
Lam  i  e     -> Node sLAM [eRT (i:env) db e]
Let  bs e     -> Node sLET (map (bRT (ids bs:env) db) bs ++
                                 eRT (ids bs:env) db  e
Case e i alts -> Node sCASE (eRT    env  db  e :
                        map (aRT (i:env) db) alts)
```

Patterns and bindings are handled in a similar way:

```
aRT :: [Local] -> [[Global]] -> Alt -> RoseTree
aRT env db alt = case alt of
  (DataAlt _, vs, e) -> eRT (vs ++ env) db e
  (LitAlt  _, _,  e) -> eRT env db e
  (Default,   _,  e) -> eRT env db e

bRT :: [Local] -> [[Global]] -> Bind -> RoseTree
bRT env db b = case b of
  NonRec i e -> eRT env db e
  Rec es     -> Node sREC (map (eRT env db . snd) es)
```

The result of eRT is a RoseTree whose branching structure mimics that of our original expression. We next need to convert this to a *matrix* of features, which we do by converting each level of the RoseTree into a row of the matrix (using pad to ensure a consistent size). Finally we turn the matrix into a *feature vector* by concatenating the rows:

```
level :: Int -> RoseTree -> [Feature]
level 0 (Node x xs) = [x]
level n (Node x xs) = concatMap (level (n-1)) xs

rt :: [[Global]] -> Expr -> [Feature]
rt db e = concat (pad cols (map (‘level‘ eRT [] db e) [0..rows]))
```

Notice that this algorithm contains several parameters, including rows and cols which determine how to truncate the matrices (defaults are 30). The kMeans function also contains a parameter for the cluster number; we set this as $\sqrt{n}$ where $n$ is the number of feature vectors being clustered.

Most of the work carried out so far has been either preliminary investigations, to determine if a particular approach is worth pursuing; or at an infrastructure level to support experimentation.

## 4.2 ML4HS

ML4HS is our top-level theory exploration framework, combining AstPlugin and MLSpec, described below, with an implementation of our recurrent clustering algorithm and the Weka machine learning library.

## 4.3 ASTPlugin

The Glasgow Haskell Compiler provides mechanisms for parsing Haskell code into tree structures, and a *renaming* transformation which makes all names unique; either by prefixing them with the name of the module which defines them, or by suffixing the name with a number. This allows us to spot repeated use of a term, across multiple modules and packages, with a simple syntactic equality check.

Since we are interested in comparing definitions based on the terms they reference, building our framework on top of GHC seems like a promising approach. Indeed, HipSpec already invokes GHC's API to obtain the definitions of Haskell functions, in order to transform them into a form suitable for ATP systems. However, our initial experiments showed that this technique is too fragile for use on many real Haskell projects.

This is due to many projects having a complex module structure, requiring particular GHC flags to be given, or using pre-processors such as `cpp` and Template Haskell to generate parts of their code. All of this complexity means that invoking GHC "manually" via its API is unlikely to obtain the definitions we require.

Thankfully there is one implementation detail which most Haskell packages agree on: the Cabal build system. All of the above complexities can be specified in a package's "Cabal file", such that the `cabal configure` and `cabal build` commands are very likely to work for most packages, without any extra effort. This shifted our focus to augmenting GHC and Cabal, such that definitions can be collected during the normal Haskell build process.

GHC provides a plugin mechanism for manipulating its Core representation, intended for optimisation passes, which we use to inspect definitions as they are being compiled. We provide a plugin called AstPlugin which implements an optimisation pass which returns its argument unchanged, but which also emits a serialised version of the definition to the console.

There are several complications in the implementation of AstPlugin. We are working with Core, which as a variant of System $F_C$ [64] has slightly different syntax and semantics to Haskell. This is mostly a benefit, since Core is a much simpler language than Haskell and its representation is relatively stable compared to many existing representations of Haskell (which often change to support various language extensions). Three areas which make Core more difficult to handle are:

Type variables: In §2.1 we saw that parametric polymorphism can be thought of as values being parameterised by type-level objects. In System F, this is represented explicitly by a special binding form $\Lambda$, distinct from the $\lambda$ binding form for value parameters. Core also has explicit bindings for type-level objects, although for simplicity it uses the same $\lambda$ representation for both types and values. This difference from Haskell, which only has explicit binding of values, alters function properties like arity.

Unified namespace: Haskell has distinct namespaces for values, types, data constructors, etc. Since Core does not make these distinctions, names may become ambiguous. For example, a type parameter `t` may be confused with a function argument `t`. To prevent this, overlapping namespaces are distinguished by prefices which are distinct from the available names; for example a type class constraint `Ord t` may give rise to a binder $\lambda$ `$dOrd` in Core. This causes difficulties when looking up names, as these prefixed forms do not easily map back to the Haskell source.

Violating encapsulation: As discussed in §2.1, Haskell allows names to be *private* to a module. When compiling Core, we have full access to private definitions, as well as references to private names from within other definitions. Hence the definitions we receive from AstPlugin will include private values which we cannot import into a theory exploration tool.

In practice, we work around these issues with a post-processing stage: for each named definition appearing in the output of AstPlugin, we attempt to type-check a Haskell expression which imports that name and passes it to QuickSpec. Those which fail, due to the reasons above and others, are discarded.

The result of building a Haskell package with AstPlugin is a database of Haskell definitions, similar in some respects to Hoogle. Definitions are indexed by a combination of their package name, module name and binding name. The definitions themselves are s-expressions representing the Core AST, with non-local references replaced by a combination of package name, module name and binding name (AKA database keys). Each definition also has an associated arity and type, obtained during the post-processing step mentioned above.

Such data is useful for multiple purposes:

- Dependency tracking: We have a tool which annotates each definition with its dependencies, i.e. those (package, module, name) combinations which it references. Definitions are then topologically sorted into dependency order, as this is required for our recurrent clustering technique.

- Machine learning: The Core s-expressions are used as input to our machine learning approaches, for guiding theory exploration using statistical properties of the theory being explored. As mentioned in §2.4.1, it is inefficient to apply intensive machine learning algorithms directly to high-dimensional data representations, so we use various feature extraction algorithms to reduce their dimensionality.

- Theory exploration: The MLSpec tool, described below, uses the output of AstPlugin to construct theories suitable for QuickSpec to explore.

- Reflection: As mentioned above, HipSpec uses the GHC API to obtain definitions of Haskell terms, which are then converted for use by theorem provers. Although we have not yet investigated this use, it seems likely that the output of AstPlugin would provide a more comprehensive and robust alternative to the GHC API approach.

- Counterexample Generation: As mentioned in §2.2, there are many Haskell property checkers, which differ mostly in the way they generate values for testing. Since our theory exploration tools are built on these property checkers, we rely on the existence of value generators for at least some of the types in our theory; yet existing approaches to deriving such generators (e.g. as found in the `derive` package) rely on choosing an arbitrary constructor then recursing. As demonstrated in §2.1, a type's constructors might not be exported, in which case these methods fail. Also, the exponential complexity of such naive recursion makes these generators unusable in many cases. It seems that a database of inspectable Haskell functions may be useful for solving this problem in a more practical way, although we have not yet performed experiments in this area.

## 4.4 MLSpec

When investigating heuristic methods like those of machine learning, it is important to use as much realistic data as possible to predict the system's performance on real tasks. One bottleneck for theory exploration is the lack of theories which are available to explore: we must manually select a set of terms to explore, and sometimes specify variables too.

Our MLSpec tool can automatically build theories suitable for exploration by QuickSpec, based on the databases constructed by AstPlugin described above. Features of MLSpec include:

- Monomorphising: Given values of polymorphic type, e.g. `safeHead :: forall t. [t] -> Maybe t` and `[] :: forall t. [t]`, a testing-based system like QuickSpec is unable to evaluate expressions such as `safeHead [] :: forall t. Maybe t` without instantiating the variable `t` to a specific type. Such an instantiation is called *monomorphising*, and in the case of MLSpec we build on previous work in QuickCheck by attempting to instantiate all type variables to `Integer`. We discard those cases where this is invalid, such as variable *type constructors* (e.g. `forall c. c Bool -> c Bool`) or incompatible class constraints (e.g. `forall t. IsString t => t`).

- Qualification: All names are *qualified* (prefixed by their module's name), to avoid most ambiguity. There is still the possibility that multiple packages will declare modules of the same name, in which case the exploration process will abort.

- Variable definition: Once a QuickSpec theory has been defined containing all of the given terms, we inspect the types it references and append three variables for each to the theory (enough to discover laws such as associativity, but not too many to overflow the limit of QuickSpec's exhaustive search).

- Sandboxing: MLSpec is built on top of `nix-eval`, which allows the theory being explored to reference packages which aren't yet installed on the system.

## 4.5 `nix-eval`

To facilitate theorem proving and machine learning, our theory exploration experiments require access to the *definitions* of the terms under investigation. This is difficult, as many terms are functions, which Haskell does not let us inspect. This limitation can be worked around by programming at a meta-level: manipulating *representations* of Haskell expressions, rather than the expressions themselves. To retain our ability to *evaluate* expressions, we then need a mechanism to transform these representations into the expressions they represent; this usually takes the form of an `eval` function.

`eval` is a common feature in languages such as Python and Javascript, where extra source files can be imported dynamically. In that case `eval` can be implemented easily by representing expressions as strings, then treating those strings as if they were the content of a file being imported.

On the other hand, Haskell does not natively support dynamic importing of extra source files, making implementation of `eval` trickier. Comprehensive implementations do exist, such as `hint`, which are effectively wrappers around GHC, but all are limited to using the Haskell modules which are already installed on the system. Since we want to explore *arbitrary* Haskell code, this is not enough for our purposes.

We have implemented a library called `nix-eval`, which provides an `eval` function for Haskell expressions which may reference packages that are not installed on the system. These packages will be automatically downloaded and installed into a sandbox when a call to `eval` is forced.

`nix-eval` is build on top of the Nix package manager and GHC. Nix provides a language for defining packages, a `cabal2nix` tool for generating Nix package definitions from those of Haskell's Cabal tool, and a `nix-shell` tool for evaluating arbitrary shell commands in a sandbox containing arbitrary packages.

The internal representation of `nix-eval` includes a list of package names, a list of module names, a list of GHC options and a string containing Haskell code. When evaluated, `nix-shell` is invoked to create a sandbox containing an instance of GHC and the Haskell packages listed in the expression. GHC is invoked in this sandbox using the `runhaskell` command, along with any options given in the expression. The code to be evaluated is prepended with `import` statements for each required module, and wrapped in a simple `main` function for printing the result of its evaluation to standard output. The expression, therefore, must have type `String`; although this is not enforced statically.

The type of the `eval` function is `Expr -> IO (Maybe String)`, where `Expr` is the type of expressions described above. The `IO` wrapper comes from our invocation of external tools, and `Maybe String` allows us to represent failure in a clean way. The restriction of expressions to `String`s is not onerous; some concrete type is required, to communicate results from the GHC invocation, but we consider the particular choice of encoding to be out of scope for `nix-eval`. It would be a straightforward exercise to wrap our `eval` function in a generic encoding mechanism, e.g. using JSON.

## 4.6 Circular Convolution

We have investigated the reduction to a fixed-size of tree structures of the following form (where `FV` denotes a feature vector):

```
data Tree = Leaf FV
          | Branch FV Tree Tree
```

Just like in the non-recursive case, the simplest way to reduce our dimensionality is to truncate. To reduce an arbitrary `t :: Tree` to a maximum depth `d > 0`, we can use `reduceD d t` where:

```
reduceD 1 (Branch fv l r) = Leaf   fv
reduceD n (Leaf   fv)     = Leaf   fv
reduceD n (Branch fv l r) = Branch fv (reduceD (n-1) l)
                                      (reduceD (n-1) r)
```

This is simple, but suffers two problems:

- We must choose a conservatively large `d`, since we're throwing away information
- The number of feature vectors grows exponentially as `d` increases

The first problem can't be avoided when truncating, but the second can be mitigated by truncating the *width* of the tree as well, to some `w > 0`. One way to truncate the width is tabulating the tree's feature vectors, then truncating the table to `w` × `d`, as ML4PG does.

Rather than truncating our trees, we can *combine* the feature vectors of leaves into their parents, and hence *fold* the tree up to any finite depth. Following [70] we have investigated the use of *circular convolution* (`cc`) as our combining function. Hence, to reduce `t :: Tree` to a single feature vector, we can use `reduceC t` where:

```
reduceC (Leaf fv)       = fv
reduceC (Branch fv l r) = cc fv (cc (reduceC l) (reduceC r))
```

Circular convolution has the following desirable properties:

Non-commutative: `cc a b` $\not\approx$ `cc b a`, hence we can distinguish between `Branch fv a b` and `Branch fv b a`

Non-associative: `cc a (cc b c)` $\not\approx$ `cc (cc a b) c`, hence we can distinguish between `Branch v1 a (Branch v2 b c)` and `Branch v1 (Branch v2 a b) c)`.

Here we use $\not\approx$ to represent that these quantities differ *with high probability*, based on empirical testing. This is the best we can do, since the type of combining functions `(FV, FV) -> FV` has a co-domain strictly smaller than its domain, and hence it must discard some information. In the case of circular convolution, the remaining information is spread out among the bits in the resulting feature, which is known as a *distributed representation* [52].

Distributed representations mix information from all parts of a structure together into a fixed number of bits, storing an *approximation* whose accuracy depends on the size of the value and the amount of storage used.

### 4.6.1 Extracting Features from XML

This method of folding with circular convolution has been implemented in the Haskell program Tree Features [8]. The feature is then:

$$feature(n) = 2^{\text{MD5}(s)} \pmod{L} \tag{3}$$

Where MD5 is the MD5 hash algorithm and $L$ is the length of the desired vector, given as a commandline argument. The result of $feature(s)$ is a bit vector of length $L$, containing only a single 1. Due to the use of a hashing function, the position of that 1 can be deterministically calculated from the input $s$, yet the *a priori* probability of each position is effectively uniform.

In other words, the hash introduces unwanted patterns which are *theoretically* learnable, but in practice a strong hash can be treated as irreversible and hence unlearnable.

### 4.6.2 Application to Coq

Prior to 2014-09-08, the Coq proof assistant provided a rudimentary XML import/export feature, which we can use to access tree structures for learning. We achieve this by using the `external` primitive of the Ltac tactic language: `external "treefeatures" "32" t1 t2 t3.` will generate an XML tree representing the Coq terms `t1`, `t2` and `t3`, and send it to the standard input of a `treefeatures` invocation, using a vector length argument of 32.

Coq will also interpret the standard output of the command, to generate terms and tactics. This functionality isn't yet used by Tree Features, but it is clear that a feedback loop can be constructed, allowing the construction of powerful Ltac tactics which invoke external machine learning systems.

# 5 Related Work

## 5.1 Haskell

Haskell is a convenient choice for our purposes for several reasons. Here we discuss the relevant language features from a high-level:

Functional: All control flow is performed by function abstraction and application, which we can reason about using standard rules of inference such as *modus ponens*.

Pure: Execution of actions (e.g. reading files) is separate to evaluation of expressions; hence our reasoning can safely ignore complicated external and non-local interactions.

[8] Available online at http://chriswarbo.net/tree-features. The application parses arbitrary trees of XML and uses binary features, ie. feature vectors are bit vectors.

To calculate the initial feature of an XML element, before any folding occurs, we concatenate its name and attributes to produce a string

Statically Typed: Expression are constrained by *types*, which can be used to eliminate unwanted combinations of values, and hence reduce search spaces; *static* types can be deduced syntactically, without having to execute the code.

Non-strict: If an evaluation strategy exists for $\beta$-normalising an expression (i.e. performing function calls) without diverging, then a non-strict evaluation strategy will not diverge when evaluating that expression. This is rather technical, but in simple terms it allows us to reason effectively about a Turing-complete language, where evaluation may not terminate. For example, when reasoning about *pairs* of values `(x, y)` and projection functions `fst` and `snd`, we might want to use an "obvious" rule such as $\forall$`x y`, `x` = `fst (x, y)`. Haskell's non-strict semantics makes this equation valid; whilst it would *not* be valid in the strict setting common to most other languages, where the expression `fst (x, y)` will diverge if `y` diverges (and hence alter the semantics, if `x` doesn't diverge).

Algebraic Data Types: These provide a rich grammar for building up user-defined data representations, and an inverse mechanism to inspect these data by *pattern-matching*. For our purposes, the useful consequences of ADTs and pattern-matching include their amenability for inductive proofs and the fact they are *closed*; i.e. an ADT's declaration specifies all of the normal forms for that type. This makes exhaustive case analysis trivial, which would be impossible for *open* types (for example, consider classes in an object oriented language, where new subclasses can be introduced at any time).

Parametricity: This allows Haskell *values* to be parameterised over *type-level* objects; provided those objects are never inspected. This has the *practical* benefit of enabling *polymorphism*: for example, we can write a polymorphic identity function `id :: forall t. t -> t`. [9] Conceptually, this function takes *two* parameters: a type `t` *and* a value of type `t`; yet only the latter is available in the function body, e.g. `id x = x`. This inability to inspect type-level arguments gives us the *theoretical* benefit of being able to characterise the behaviour of polymorphic functions from their type alone, a technique known as *theorems for free* [65].

Type classes: Along with their various extensions, type classes are interfaces which specify a set of operations over a type (or other type-level object, such as a *type constructor*). Many type classes also specify a set of *laws* which their operations should obey but, lacking a simple mechanism to enforce this, laws are usually considered as documentation. As a simple example, we can define a type class `Semigroup` with the following operation and associativity law:

```
op :: forall t. Semigroup t => t -> t -> t
```

[9] Read "`a :: b`" as "`a` has type `b`" and "`a -> b`" as "the type of functions from `a` to `b`".

$$\forall \texttt{x y z}, \texttt{op x (op y z)} = \texttt{op (op x y) z}$$

The notation `Semigroup t =>` is a *type class constraint*, which restricts the possible types `t` to only those which implement `Semigroup`. [10] There are many *instances* of `Semigroup` (types which may be substituted for `t`), e.g. `Integer` with `op` performing addition. Many more examples can be found in the *typeclassopedia* [69]. This ability to constrain types, and the existence of laws, helps us reason about code generically, rather than repeating the same arguments for each particular pair of `t` and `op`.

Equational: Haskell uses equations at the value level, for definitions; at the type level, for coercions; at the documentation level, for typeclass laws; and at the compiler level, for ad-hoc rewrite rules. This provides us with many *sources* of equations, as well as many possible *uses* for any equations we might discover. Along with their support in existing tools such as SMT solvers, this makes equational conjectures a natural target for our investigation.

Modularity: Haskell has a module system, where each module may specify an *export list* containing the names which should be made available for other modules to import. When such a list is given, any expressions *not* on the list are considered *private* to that module, and are hence inaccessible from elsewhere. This mechanism allows modules to provide more guarantees than are available just in their types. For example, a module may represent email addresses in the following way:

```
module Email (Email(), at, render) where

data Email = E String String

render :: Email -> String
render (E u h) = u ++ "@" ++ h

at :: String -> String -> Maybe Email
at "" h  = Nothing
at u  "" = Nothing
at u  h  = Just (E u h)
```

The `Email` type guarantees that its elements have both a user part and a host part (modulo divergence), but it does not provide any guarantees about those parts. We also define the `at` function, a so-called "smart

[10] Alternatively, we can consider `Semigroup t` as the type of "implementations of `Semigroup` for `t`", in which case `=>` has a similar role to `->` and we can consider `op` to take *four* parameters: a type `t`, an implementation of `Semigroup t` and two values of type `t`. As with parametric polymorphism, this extra `Semigroup t` parameter is not available at the value level. Even if it were, we could not alter our behaviour by inspecting it, since Haskell only allows types to implement each type class in at most one way, so there would be no information to branch on.

constructor", which has the additional guarantee that the `Emails` it returns contain non-empty `Strings`. By ommitting the `E` constructor from the export list on the first line [11], the only way *other* modules can create an `Email` is by using `at`, which forces the non-empty guarantee to hold globally.

Together, these features make Haskell code highly structured, amenable to logical analysis and subject to many algebraic laws. However, as mentioned with regards to type classes, Haskell itself is incapable of expressing or enforcing these laws (at least, without difficulty [37]). This reduces the incentive to manually discover, state and prove theorems about Haskell code, e.g. in the style of interactive theorem proving, as these results may be invalidated by seemingly innocuous code changes. We will revisit the second-class status of theorem proving in Haskell in our discussion of theory exploration (§2.3), but we will remark that Haskell is thus in a unique position with regards to the discovery of interesting theorems. Namely that many discoveries may be available with very little work, simply because the code's authors are focused on *software* development rather than *proof* development. The same cannot be said, for example, of ITP systems; although our reasoning capabilities may be stronger in an ITP setting, much of the "low hanging fruit" will have already been found through the user's dedicated efforts, and hence TE would be more likely to fit into an automation role for the user, rather than providing truly unexpected new discoveries.

Other empirical advantages to studying Haskell, compared to either other programming languages or theorem proving systems, include:

- The large amount of Haskell code which is freely available online, e.g. in repositories like Hackage, with which we can experiment.
- The existence of conjecture generation and theory exploration systems for Haskell, such as QuickSpec and HipSpec, and counterexample finders like QuickCheck, SmallCheck and SmartCheck.
- The remarkable amount of infrastructure which exists for working with Haskell code, including package managers, compilers, interpreters, parsers, static analysers, etc.

## 5.2 Relevance Filtering

[33]

The combinatorial nature of formal systems causes many proof search methods, such as resolution, to have exponential complexity [19]; hence even a modest size increase can turn a trivial problem into an intractable one. Finding efficient alternatives for such algorithms, especially those which are NP-complete (e.g. determining satisfiability) or co-NP-complete (e.g. determining tautologies),

[11] The syntax `Email()` means we're exporting the `Email` type, but not any of its constructors.

seems unlikely, as it would imply progress on the famously intractable open problems of P = NP and NP = co-NP. On the other hand, we can turn this difficulty around: a modest *decrease* in size may turn an intractable problem into a solvable one. We can ensure that the solutions to these reduced problems coincide with the original if we only remove *redundant* information. This leads to the idea of *relevance filtering*.

Relevance filtering simplifies a proof search problem by removing from consideration those clauses (axioms, definitions, lemmas, etc.) which are deemed *irrelevant*. The technique is used in Sledgehammer during its translation of Isabelle/HOL theories to statements in first order logic: rather than translating the entire theory, only a sub-set of relevant clauses are included. This reduces the size of the problem and speeds up the proof search, but it creates the new problem of determining when a clause is relevant: how do we know what will be required, before we have the proof?

The initial approach, known as MePO (from *Meng-Paulson* [43]), gives each clause a score based on the proportion $m/n$ of its symbols which are "relevant" (where $n$ is the number of symbols in the clause and $m$ is the number which are relevant). Initially, the relevant symbols are those which occur in the goal, but whenever a clause is found which scores more than a particular threshold, all of its symbols are then also considered relevant. There are other heuristics applied too, such as increasing the score of user-provided facts (e.g. given by keywords like `using`), locally-scoped facts, first-order facts and rarely-occuring facts. To choose $r$ relevant clauses for an ATP invocation, we simply order the clauses by decreasing score and take the first $r$ of them.

Recently, a variety of alternative algorithms have also been investigated, including:

MaSH: Machine Learning for SledgeHammer [32]. The distinguishing feature of MaSH is its use of "visibility", which is essentially a dependency graph of which theorems were used in the proofs of which other theorems; although theorems are represented as abstract sets of features. To select relevant clauses for a goal, the set of clauses which are visible from the goal's components is generated; this is further reduced by (an efficient approximation of) a naive Bayes algorithm.

MOR: *Multi-output ranking* uses a support vector machine (SVM) approach for selecting relevant axioms from the Mizar Mathematical Library for use by the Vampire ATP system [1]. It compares favourably to SNoW and SInE.

SInE

BliStr

HOLyHammer

MoMM

SNoW

MPTP 0.2

MaLARea

MaLARea SG1

## 5.3 Clustering Expressions

[31] [22]

### 5.3.1 Learning From Structured Data

One major difficulty with formal mathematics as a domain in which to apply statistical machine learning is the use of *structure* to encode information in objects. In particular, *trees* appear in many places: from inductive datatypes, to recursive function definitions; from theorem statements, to proof objects. Such nested structures may extend to arbitrary depth, which makes them difficult to represent with a fixed number of features, as is expected by most machine learning algorithms. Here we review a selection of solutions to this problem, and compare their distinguishing properties.

**5.3.1.1 Truncation and Padding** The simplest way to limit the size of our inputs is to truncate anything larger than a particular size (and pad anything smaller). This is the approach taken by ML4PG [20], which limits itself to trees with at most 10 levels and 10 elements per level; each tree is converted to a $30 \times 10$ matrix (3 values per tree node) and learning takes place on these normalised representations.

Truncation is unsatisfactory in the way it balances *data* efficiency with *time* efficiency. Specifically, truncation works best when the input data contains no redundancy and is arranged with the most significant data first (in a sense, it is "big-endian"). The less these assumptions hold, the less we can truncate. Since many ML algorithms scale poorly with input size, we would prefer to eliminate the redundancy using a more aggressive algorithm, to keep the resulting feature size as low as possible.

**5.3.1.2 Dimension Reduction** A more sophisticated approach to the problem of reducing input size is to view it as a *dimension reduction* technique: our inputs can be modelled as points in high-dimensional spaces, which we want to project into a lower-dimensional space ($\{0, 1\}^N$ in the case of $N$-bit vectors).

Truncation is a trivial dimension reduction technique: take the first $N$ coordinates (bits). More sophisticated projection functions consider the *distribution* of the points, and project with the hyperplane which preserves as much of the variance as possible (or, equivalently, reduces the *mutual information* between the points).

There are many techniques to find these hyperplanes, such as *principle component analysis* (PCA) and *autoencoding*; however, since these techniques are effectively ML algorithms in their own right, they suffer some of the same constraints we're trying to avoid:

- They operate *offline*, requiring all input points up-front
- All input points must have the same dimensionality

In particular, the second constraint is precisely what we're trying to avoid. Sophisticated dimension reduction is still useful for *compressing* large, redundant features into smaller, information-dense representations, and as such provides a good complement to truncation.

The requirement for offline "batch" processing is more difficult to overcome, since any learning we perform for feature extraction will interfere with the core learning algorithm that's consuming these features (this is why deep learning is often done greedily).

**5.3.1.3 Sequencing** The task of dimension reduction changes when we consider *structured* data. Recursive structures, like trees and lists, have *fractal* dimension: adding layers to a recursive structure gives us more *fine-grained* features, rather than *orthogonal* features. For data mining context-free languages (e.g. those of programming and theorem-proving systems), we will mainly be concerned with tree structures of variable size.

Any investigation of variable-size input would be incomplete without mentioning *sequencing*. This is a lossless approach, which splits the input into fixed-size *chunks*, which are fed into an appropriate ML algorithm one at a time. The sequence is terminated by a sentinel; an "end-of-sequence" marker which, by construction, is distinguishable from the data chunks. This technique allows us to trade *space* (the size of our input) for *time* (the number of chunks in a sequence).

Not all ML algorithms can be adapted to accept sequences. One notable approach is to use *recurrent ANNs* (RANNs), which allow arbitrary connections between nodes, including cycles. Compared to *feed-forward* ANNs (FFANNs), which are acyclic, the *future output* of a RANN may depend arbitrarily on its *past inputs* (in fact, RANNs are universal computers).

The main problem with RANNs, compared to the more widely-used FFANNs, is the difficulty of training them. If we extend the standard backpropagation algorithm to handle cycles, we get the *backpropagation through time* algorithm [66]. However, this suffers a problem known as the *vanishing gradient*: error values decay exponentially as they propagate back through the cycles, which prevents effective learning of delayed dependencies, undermining the main advantage of RANNs. The vanishing gradient problem is the subject of current research, with countermeasures including *neuroevolution* (using evolutionary computation techniques to train an ANN) and *long short-term memory* (LSTM; introducing a few special, untrainable nodes to persist values for long time periods [24]).

The application of *kernel methods* to structured information is discussed in [16], where the input data (including sequences, trees and graphs) are represented using *generative models*, such as hidden Markov models, of a fixed size.

[16] [50] [5] [52] [18] [34] [53] [70]

# 6 Evaluation

TODO

Future work? Hypothetical use cases?

# 7 Future Work

## 7.1 Extensions

Our use of clustering to pre-process QuickSpec signatures necessarily involves many decisions and tradeoffs. There are many alternative approaches which are ripe for investigation:

- Improvements to our feature extraction algorithm, in particular to handle types.
- Alternative clustering algorithms.
- *Feature learning* uses machine learning algorithms in place of hand-coded feature extraction algorithms such as ours. A comparison of our hand-picked features against a selection of learned representations would be a useful indication of the importance that understanding the expression language may or may not have on identifying salient aspects of expressions.
- There are several potential alternatives to QuickCheck for instantiating variables, which may improve performance of QuickSpec by either generating expressions more efficiently (as in SmallCheck's enumeration approach) or by observing differences with fewer tests (as found in Lazy SmallCheck's demand-driven enumeration).

## 7.2 Interestingness

It is important to consider the question: *what if we succeed?* What if a more efficient theory exploration system were possible, capable of reading huge amounts of code and producing an abundance of theorems? How could the output be made manageable, by finding the needles we are interested in among the haystack of potential laws?

This is governed by the "interestingness" criteria of the theory exploration system: what to keep and what to discard, and even what areas of the search space to prioritise. QuickSpec's approach, briefly mentioned in §2.3, is very simple: we discard equations which are direct consequences of others, and keep all the rest.

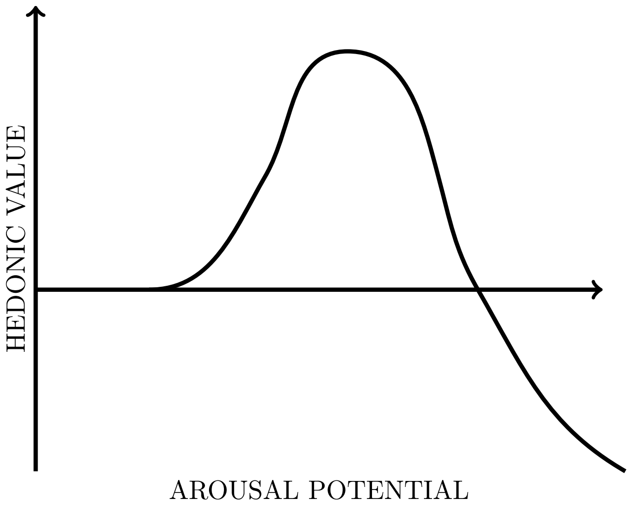


Figure 7: The Wundt curve, reproduced from [8]. The axes "hedonic value" and "arousal potential" are described as covering "reward value. . . preference or pleasure", and "all the stimulus properties that tend to raise arousal, including novelty and complexity", respectively.

### 7.2.1 Interestingness in Concept Formation

[45] [51] [68] [14] [15] [13] [36] [46] [10] [28] [62] [13] [17]

### 7.2.2 Artificial Curiosity

*Artificial curiosity* (AC) describes active learning systems which are rewarded based on how interesting the input or data they discover is [60]. Although framed in the context of *reinforcement learning*, this is clearly relevant to our theory exploration setting.

As an unsupervised learning task, AC has no access to labels or meanings associated with its input; the only features it can learn are the structure and relationships inherent in the data, which is very much what we would like a theory exploration system to do. The unifying principle of AC methods is to force systems away from inputs which are not amenable to learning; either because they are so familiar that there is nothing left to learn, or so unfamiliar that they are unintelligible. The resulting behaviour is characterised by the *Wundt curve* (shown in figure 7) [12], which has been used in psychology to explain human aesthetics and preferences [8].

We can divide AC approaches into two groups: the first, which we call *explicit*, send inputs which follow a Wundt curve to their learning algorithm; the second, the *implicit* approaches, instead modify the *output* of their learning

[12] In practice, many measures avoid negative values for simplicity, in which cases we replace all negative points on the curve with zero.

algorithm(s), such that the overall system follows a Wundt curve as an emergent property.

In the explicit case, the *implicit reward* signals being learned are analogous to our notion of interestingness. A framework encompassing many examples is given in [48] in the context of reinforcement learning.

One particularly general measure is *compression progress*: given a compressed representation of our previous observations, the "progress" is the space saved if we include the current observation. Observations which are incompressible or trivially compressible don't save any space, whilst observations which provide new information relevant to past experience can provide a saving. This can be translated to a theorem proving context very naturally: our observations are theorems and their proofs, whilst new theorems which generalise known results will allow us to compress their proofs.

[59]

Two sources of intrinsic reward are proposed in [23] for *random forests*. A random forest is a population of decision trees, where each tree is trained on a sub-set of the available examples, each decision is made using a sub-set of the available features, and the predictions of every tree are averaged to obtain that of the forest [9]. The first intrinsic reward is the *disagreement* between predictions; for a forest with $m$ models (trees), predicting features $x_1 \dots x_n$ of the state resulting from taking action $a$ in state $s$, we simply sum the Kullback-Leibler divergence $D_{\text{KL}}$ of each prediction $P_1 \dots P_m$ from every other prediction:

$$D(s,a) = \sum_{i=1}^{n} \sum_{j=1}^{m} \sum_{k=1}^{m} D_{KL}(P_j(x_i|s,a)||P_k(x_i|s,a)) \tag{4}$$

$D(s,a)$ is an explicit AC reward, as it follows a Wundt curve as the complexity of transitions increases. For parts of the state space which have been fully learned, the models will agree on accurate predictions. For parts which are unlearnable, the models cannot infer any structure, and will converge to reporting the average of past observations; these predictions may not be accurate, but they will be in agreement. Hence it is the states which are amenable to learning which produce the largest disagreement.

The second intrinsic reward is simply a measure of distance from previous observations, which pushes the system towards unseen states regardless of how learnable they are (similar to the $R_{max}$ technique). This is too simple to meet our definition of AC, but it does force the models to generalise their predictions to unexplored states, acting to increase disagreement in the forest.

A key advantage of random forests is that their models are *inspectable*: they not only give predictions, but also *reasons* for those predictions (i.e. we can see which paths are taken through each decision tree).

[30] [38] [39] [40] [54] [55] [57] [59] [58] [61] [63] [41] [44] [47] [49] [60]

Whilst clearly of relevance to theory exploration, artificial curiosity is usually framed in the context of a *reinforcement learning* and *intrinsic reward*, especially in the field of developmental robotics. This requires non-trivial choices to be made in deciding which of its concepts are of relevance to our domain, and how they may be translated across. For example, much of developmental robotics studies continuous, real-valued sensorimotor signals which may not have any direct analogue in the manipulation of logical formulae. However, if we take a higher-level view, the study of such signals may provide insight for predicting and tuning the behaviour of off-the-shelf ATP algorithms.

The most obvious contrast between developmental robotics and theory exploration is that the latter is not physically embodied (e.g. in a robot). Embodiment has been proposed as a necessary property of intelligent systems, as it provides *grounding* [2]. Embodiment emerged as a response to the symbolic techniques of GOFAI, and in this sense the fields of theory exploration and developmental robotics seem incompatible. Nevertheless, TE can be seen to avoid the problems of GOFAI in two ways:

- Firstly, the abstract, mathematical domain being explored is not a *model* of some external, physical environment; the domain *is* our environment; hence there is no issue of grounding terms with some external meaning.
- Secondly, there is a physical aspect of TE in that *resource usage* is a critical factor. If it weren't, then brute force enumeration of proofs would be a viable solution. In this sense, we can provide physical inputs to our algorithms, such as measures of time and space used.

### 7.2.3 Interestingness in Evolutionary Computation

*Evolutionary computation* is an umbrella term for heuristic search algorithms which mimic the process of evolution by natural selection among a population of candidate solutions [4]. Whilst *genetic algorithms* are perhaps the most well-known instance of evolutionary computation, their use of *strings* to represent solutions causes complications when comparing to a domain like theory exploration, where recursive structures of unbounded depth arise. Thankfully these problems are not insurmountable, for example *genetic programming* can operate on tree-structures natively [6], which makes evolutionary computation a useful source of ideas for reuse in our theory exploration setting.

Traditionally, evolutionary approaches assign solutions a *fitness* value, using a user-supplied *fitness function.* Fitness should correlate with how well a solution solves the user's problem; for example, the fitness of a solution to some engineering problem may depend on the estimated materials cost. If we frame the task of theory exploration in evolutionary computation terms, the fitness function would be our interestingness measure.

Pure exploration (i.e. for its own sake) has been studied in evolutionary computation for two main reasons: *artificial life* and *deceptive problems.* The former attempts to gain insight into the nature of life and biology through competition over limited resources. Whilst this may have utility in resource allocation, e.g. efficient scheduling of a portfolio of ATP programs, there is no direct connection to interestingness in theory exploration, so we will not consider it further (note that similar resource-usage ideas can also be found in the literature on *artificial economies*, e.g. [7]).

On the other hand, work on deceptive problems is highly relevant, as it has lead to studying various notions of intrinsic fitness, which are analogous to the interestingness measures we want. Deceptive problems are those where "pursuing the objective may prevent the objective from being reached" [35], which is caused by the fitness (objective) function having many local optima which are easy to find (e.g. by hill climbing), but few global optima which are hard to find. Many approaches try to avoid deception by augmenting the given fitness function to promote *diversity* and *novelty*, such as *niching methods* [56].

One example is *fitness sharing*, which divides up fitness values between identical or similar solutions. Say we have a user-provided fitness function $f$, and a population containing two identical solutions $s_1$ and $s_2$; hence $f(s_1) = f(s_2)$. In a fitness sharing scheme, we interpret fitness as a fixed resource, distributed according to $f$; when multiple individuals occupy the same point in the solution space, they must *share* the fitness available there. We can describe the fitness *allocated* to a solution by augmenting $f$, e.g. if we allocate fitness uniformly between identical solutions we get:

$$f'(x) = \frac{f(x)}{\sum_{i=1}^{n} \delta_{s_i x}}$$

Where $n$ is the population size, $s_i$ is the $i$th solution in the population and $\delta$ is the Kronecker delta function. In the example above, assuming there are no other copies in the population, then $f'(s_1) = \frac{f(s_1)}{2} = \frac{f(s_2)}{2} = f'(s_2)$. By sharing in this way, the fitness of each solution is balanced against redundancy in the population: there may still be many copies of a solution, but only when the fitness is high enough to justify all of them.

There are many variations on this theme, such as sharing between "close" solutions rather than just identical ones and judging distance based on fitness (AKA phenotypically) rather than based on the location in solution space (AKA genetically). Yet the underlying principle is always the same: penalise duplication in order to promote diversity. This lesson can be carried over to our theory exploration context, where a theorem should be considered less interesting if it is "close" to others which have been found.

In a similar way, we can bias our search procedure, rather than our fitness function, towards diversity. The search procedure in population-based evolutionary algorithms consists of *selecting* one or more individuals from the population, e.g. via truncation (select the best $n$ individuals, discarding the rest); then *transforming* the selected individuals, e.g. via mutation and crossover, to obtain new solutions.

Traditional selection methods are biased towards high fitness individuals (this is especially clear for truncation). Alternative schemes have been proposed which favour diversity *at the expense of* fitness. For example, the fitness uniform selection scheme (FUSS) [26] selects a target fitness $f_t$ uniformly from the interval $[f_{min}, f_{max}]$ between the highest and lowest of the population. An individual $s$ is then selected with fitness closest to $f_t$, i.e. $s = \underset{x}{\text{argmin}}|f(x) - f_t|$

In this way, the fitness function $f$ is used to assign comparable quantities to solutions, but it is not treated as the objective; instead, the implicit objective is to maintain a diverse population, with individuals spread out uniformly in fitness space. This approach seems useful for informing our work in theory exploration, as it supports search criteria which *describe* solutions, but which we may not want to *optimise*. As a simple example, we might distinguish different forms of theorem by measuring how balanced their syntax trees are (-1 for left-leaning, +1 for right leaning, 0 for balanced); but it would be senseless to *maximise* how far they lean.

Once we begin this process of augmenting fitness functions, or abandoning their use as objectives, an obvious question arises: what happens if our new function contains nothing of the original? This kind of pure exploration scenario leads to a variety of ideas for *instrinsic* fitness, such as novelty [35], which can lead to learning useful "stepping stones" even in objective-driven domains. Such intrinsic notions of fitness are direct analogues of the interestingness measures we seek for theory exploration.

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