

Interestingness Measures for Theory Exploration

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October 30, 2015

Abstract

Since their inception, computers have been applied to automate and assist work in mathematics, with established fields including numerical computation, computer algebra, (online) communication and so on. Here we focus on their use in two areas: formal proof and statistics; and how new approaches are bringing these seemingly disparate disciplines closer together.

1 Introduction

As computers and software become more capable, 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. Mathematics provides us with powerful, systematic methods of reasoning, which we can bring to bear on this challenge; in particular those of *formal logic* and *statistics*. By (partially) mechanising these approaches, in the fields of *theorem proving* and *machine learning*, respectively, we can leverage these increasing machine capabilities and direct them for the purpose of analysis. However, the question still remains: on what should we focus that analysis?

In this work, we investigate the notion of *interestingness* in the exploration of formal systems (an area known as *theory exploration*) as a way to make productive use of resources in an often intractable domain. To keep things concrete, we focus our formal analysis on equational formulae describing programs in the Haskell language, for reasons elaborated in §2.1. Conceptually, we maintain a broader view, and survey many related areas which may offer insights on the problem.

Appeals to interestingness arise when more direct measures, such as utility, are not available. For example, the inclusion of particular statements in a program or proof development can be easily justified based on their contribution to the overall solution; however, in a *library* there is no particular problem being solved, in which case we must judge statements on less direct criteria, such as

how “interesting” they may be to our users. Appeals to interestingness abound in the history of computer-assisted reasoning; for example, in 1971 Plotkin [66] considered the task of “discovering theorems T from a system of axioms Ax ”, and in particular the questions “Under what conditions is T an interesting, possible theorem in the system Ax ?” and “Is there a way to generate (most) interesting possible theorems?”. Despite such widespread use of the term, there is no standard definition of what makes a formal object, whether it is an axiom, a conjecture, a proof, etc., “interesting”; although many ad-hoc heuristics have been proposed.

We begin our undertaking in §2 by introducing the Haskell language, as well as the relevant fields of verification for context. We define a formal framework for our investigation, and show how it relates to the existing theorem proving landscape. A selection of theorem proving scenarios which *require* exploration are discussed in §3, whilst related work, including existing definitions of interestingness, is surveyed in §4. We also review the use of exploration in other fields of Artificial Intelligence and Machine Learning, where researchers are experimenting with replacing *explicit* goals and rewards with *implicit* alternatives such as interestingness. Recent efforts in this area have led to the emergence of principled theories, mostly based around (algorithmic) information theory, which may be adapted to our theory exploration context.

We discuss our present contributions in §5 and future research directions in §6, before concluding in §7.

2 Background

Most work in mechanised, formal mathematics focuses on a *theorem proving* paradigm, usually either *interactive theorem proving* (ITP) or *automated theorem proving* (ATP). Whilst the boundaries between these approaches can be somewhat blurred, we give precise definitions in §2.2 and §2.3, respectively, and characterise both as being *goal-driven*: particular conjectures must be provided as input to the process, and the output is either a proof, a refutation or “don’t know” (in the case of incomplete procedures).

In this work, we instead adopt the paradigm of *(automated) theory exploration*, discussed in §2.4, which includes the ability to *generate* conjectures, and hence output *novel* theorems. Since many theories will admit an infinite number of trivial theorems (e.g. \top , $\top \wedge \top$, $(\top \wedge \top) \wedge \top$, ...) we require some mechanism for avoiding such undesirable, yet provable, statements. This is the role of interestingness, which we can use to *judge* a statement, in a potentially rich way, rather than merely constructing or failing to construct a proof.

Firstly, however, we give an overview of the Haskell programming language in §2.1. This allows us to establish many concepts in a straightforward software context, which we can then re-use in the potentially less-familiar realm of interactive theorem proving. We decided to focus on Haskell as it has mature, state-of-the-art theory exploration implementations (QUICKSPEC [18] and HIP-SPEC [17]). This is evident from the fact that the state-of-the-art equivalent for

Isabelle/HOL, the HIPSTER [35] system, is actually implemented by translating to Haskell and invoking HIPSPEC.

2.1 Haskell

Haskell is a programming language which is well-suited to research; indeed, this was a goal of the language’s creators [49]. Like most members of the *functional programming* paradigm, Haskell is essentially a variant of λ -calculus; in fact the GHC compiler uses (variants of) the polymorphic λ -calculus *System F* as an intermediate representation (referred to as *GHC Core*). For a detailed exposition of the language syntax and semantics, you can consult the Haskell Language Report [49]¹ or a textbook such as [83]; here we will focus on those language features which make it particularly suited for our formal reasoning purposes:

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.

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 β -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 $\forall x y, x = \mathbf{fst} \ (x, y)$. 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

¹Version 2010 was current as this was written

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`.² 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* [84].

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:

$$\text{op} :: \text{forall } t. \text{Semigroup } t \Rightarrow t \rightarrow t \rightarrow t$$

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

The notation `Semigroup t =>` is a *type class constraint*, which restricts the possible types `t` to only those which implement `Semigroup`.³ 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* [89]. 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.

²Read “`a :: b`” as “`a` has type `b`” and “`a -> b`” as “the type of functions from `a` to `b`”.

³Alternatively, 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.

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 [44]). This reduces the incentive to manually discover, state and prove theorems about Haskell code, e.g. in the style of interactive theorem proving (see §2.2), 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 (§2.4), 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.

2.2 Interactive Theorem Proving

ITP is based around a *proof checker* C , which is a decision procedure for determining if a given value P (known as a *proof object* or *witness*) constitutes a proof of a given statement S :

$$C: (P \times S) \rightarrow \text{Boolean}$$

The process of ITP can hence be understood as the search for an appropriate P for our *goal* S :

$$\text{ITP}: (S \times C) \rightarrow \{P \mid C(P, S) = \text{True}\}$$

It just so happens that a useful way to implement such a system is via pure functional programming, with the result that many ITP systems (AKA *proof assistants*) such as Coq and Agda appear very similar to languages like Haskell. In particular, we can represent statements S as types and proofs P as values,

in which case the proof checker C is simply a type-checker. There are some obvious quirks, such as the need to be *total* (not Turing-complete) in order to ensure soundness, but overall many of the features we introduced for Haskell, such as parametricity, type classes and ADTs are directly translatable to the ITP setting.

This coincidence is due to the *Curry-Howard correspondence* [85], which identifies programming languages with systems of logic. Functional programming languages correspond to intuitionistic logics, and are hence a natural fit for reasoning on computers. With additional axioms, we can extend these to more familiar classical logics, although these can make it harder to compute.

Most differences between functional programming and ITP stem from different *expectations* of the user. In the case of Haskell, the desire for expressivity outweighs the desire for soundness, and hence its designers opted to make it Turing-complete. For an ITP language like Agda, soundness far outweighs the inconvenience of having to prove termination, so the opposite tradeoff is made. Similarly, since many ITP “programs” (proofs) will never be executed, the language can avoid optimisation in favour of simplicity (and hopefully correctness). This approach is summed up by the *de Bruijn criterion*, which requires that the system “generates ‘proof-objects’ (of some form) that can be checked by an ‘easy’ algorithm” [7, § 2]. One nice consequence of this approach, which is followed for example by Isabelle [58] and Coq [10], is that the proof assistants themselves can become arbitrarily complex and even buggy, yet as long as the proof checker remains simple we can maintain a high degree of confidence in the results.

Their emphasis on *interactivity*, mostly caused by operating in undecidable domains, means ITP can require an enormous effort for non-trivial proof or verification tasks (e.g. see [26]). One common way to mitigate this problem is by implementing powerful *tactics*: meta-programs which automate as much of a proof as possible. The most striking example of such meta-programming is the *Sledgehammer* component of Isabelle/HOL [51], which invokes a multitude of ATP systems on (a translated form of) the current goal to see if any can provide a proof which Isabelle’s core checker will accept.

2.3 Automated Theorem Proving

ATP systems are similar in principle to proof assistants, but are based around a *proof search* algorithm rather than a proof checker. By using a fixed algorithm for proving, such as *resolution* [73, § 9.6] or *superposition* [3], ATP programs are limited to particular decidable or semi-decidable fragments of logic. In particular, most ATP systems (such as E [79] and Vampire [70]) operate in classical first-order logic. This is the most striking difference from ITP systems (e.g. Coq, Agda and Isabelle) which operate in higher-order logics.

In addition to its interest to logicians, ATP has been actively researched in the field of artificial intelligence, dating back to the founding of the field at the 1956 Dartmouth conference. Even by that time Newell and Simon had developed their Logic Theory Machine [57], which was subsequently able to prove theorems

like those in Principia Mathematica [56]. The approaches now known as *good old-fashioned AI* (GOFAI) were due in part to the success of automated theorem proving, as attempts were made to formulate many problems in a way amenable to these powerful first-order reasoners.

Recently there has been a trend away from this direction, towards statistical formulations amenable to machine learning, which we will review in §4.

2.4 Theory Exploration

The most striking difference between theory exploration (TE) and theorem proving is the former’s lack of an explicit goal (e.g. a user-provided conjecture to prove). Instead, the *implicit* goal is more open-ended: the discovery of “interesting” conclusions from the given premises. Of course, a key question to ask is what do we mean by “interesting”? There is no single answer, although many approximate measures have been proposed. The choice of what counts as interesting has been used to classify various TE implementations [86], along with their approaches to term generation, well-formedness and proof.

Following [86], we call a pair (Σ, V) , of a signature and a set of variables, a *theory*. *Theory exploration* then refers to any process $(\Sigma, V) \xrightarrow{TE} \text{Terms}(\Sigma, V)$ for producing terms of the theory which are well-formed, provable and “interesting”.

The conditions of well-formedness and provability can be handled through the use of type systems and automated theorem provers. Hence the method of conjecture generation, and the determination of what is interesting, are the most important properties of any TE system.

Early implementations like THEOREMA [14] provided interactive environments, similar to computer algebra systems and interactive theorem provers, to assist the user in finding theorems. Like in the ITP approach, the relatively simple process of verification is automated, whilst the more difficult tasks (term generation and the determination of their interest) are left up to the user.

Subsequent systems have investigated *automated* theory exploration, for tasks such as lemma discovery [35]. By removing user interaction, these properties must be implemented by algorithms. In existing systems these are tightly coupled to improve efficiency, which makes it difficult to try different approaches independently.

As an example, QUICKSPEC [18] discovers equations about Haskell code, which are defined as “interesting” if they cannot be simplified using previously discovered equations. The intuition for such criteria is to avoid special cases of known theorems, such as $0 + 0 = 0$, $0 + 1 = 1$, etc. when we already know $0 + x = x$. Whilst this interestingness judgement is elegantly implemented with a congruence closure relation (version 1) and a term rewriting system (version 2), the conjecture generation is performed in a brute-force way.

Although QUICKSPEC only *tests* its equations rather than proving them, it is still used as the exploration component of more rigorous systems like HIPSPEC and HIPSTER.

HIPSPEC is currently the most powerful TE system for Haskell, and also

forms a major component of HIPSTER. It uses off-the-shelf ATP programs (including AltErgo, Vampire, Z3, E, SPASS and CVC4) to verify the conjectures of QUICKSPEC. QUICKSPEC, in turn, enumerates all type-correct combinations of the terms in the theory up to some depth, groups them into equivalence classes using the QUICKCHECK counterexample finder, then conjectures equations relating the members of these classes. This approach works well as a lemma generation system, making HIPSPEC a capable inductive theorem prover as well as a theory exploration system [17]. HIPSPEC is also compatible with Haskell’s existing testing infrastructure, such that an invocation of `cabal test` can run HIPSPEC alongside more traditional QA tools like QUICKCHECK, HUNIT and CRITERION.

In fact, there are similarities between the way a TE system like HIPSPEC can generalise from proving *particular* theorems to *inventing* theorems, and the way counterexample finders like QUICKCHECK can generalise from testing *particular* expressions to *inventing* expressions to test. There are likely lessons that each can learn from the other’s approach to term generation.

3 Exploration in Theorem Proving

Before exploring abstract definitions of interestingness, we can first consider some scenarios which arise during formal proof where we are forced to generate conjectures. An analysis of these situations, and the subsequent theorems they produce, will contribute towards an empirical justification for what is interesting (at least from a utilitarian point of view) and inform our later exploration of the literature.

3.1 Generalisation

When we *generalise* a statement S , we obtain a new statement S' of which S is a special case. Although it seems counterintuitive, a generalised statement can sometimes be *easier* to prove than the original. This arises often in inductive proofs, since the specific obligations which arise in the proof may be incompatible with the available inductive hypotheses.

However, we cannot blindly generalise *all* obligations we encounter, since *over-generalising* results in obligations which are so strong that they are unprovable, or even false. We must therefore rely on heuristics to guide the generation of generalised conjectures, and hence perform a kind of exploration.

An informative example is given by Boyer and Moore of the associativity of multiplication in ACL2 [12]:

$$(x * y) * z = x * (y * z)$$

During the course of the proof, the following obligation arises:

$$(y + (x * y)) * z = (y * z) + ((x * y) * z) \quad (\text{conc3})$$

ACL2 automatically generalises (conc3) by replacing the repeated sub-term $x * y$ with a fresh variable w :

$$(y + w) * z = (y * z) + (w * z) \quad (\text{conc4})$$

This generalised form is clearly the distributivity law for multiplication and addition, which can be proved separately to the original goal of associativity. It would not be controversial to claim that this distributivity law is interesting in its own right (relative to associativity, at least), in addition to its usefulness in making this proof go through.

Generalisation also occurs frequently when reasoning about *tail-recursive* definitions [37].⁴

3.2 Analogy

One way to characterise the interestingness of a statement is by *analogy* to existing interesting statements. By finding lemmas analogous to those of a different theory, we may be able to re-use tactics and other forms of meta-programming across both.

Existing theory exploration systems have been successfully applied to this problem, however the use of pure exploration misses opportunities to *focus* the search, since we know which lemmas are used in those theories where a technique succeeded. If we can find an analogy to map from such solved problems to our unsolved goal, we can infer the approximate form of the lemmas we require, and target these specifically.

The approach taken by ACL2(ML) is to find lemmas which may be relevant to solving a goal G by making analogies via unsupervised clustering [28]. These clusters are used in two ways:

- First, we use the cluster C_G containing G to identify analogous theorems.
- For each theorem $T \in C_G \setminus \{G\}$, we consider those symbols S_T which occur in T but not in G . Our analogous lemmas are those used to prove T , mutated such that symbols $s \in S_T$ are replaced by members of the cluster C_s containing s .

The running examples for demonstrating ACL2(ML) are equivalence theorems for tail-recursive and non-tail-recursive calculations, as well as the effect of repeating certain list operations:

- $\forall n, \text{natp}(n) \rightarrow \text{fact-tail}(n) = \text{fact}(n)$ where **natp** is the predicate that n is a natural number, whilst **fact-tail** and **fact** are tail-recursive and non-tail-recursive implementations of factorial, respectively.

⁴A tail-recursive function can be executed in constant space using a loop, whereas recursion in non-tail positions may require a growing number of stack frames or nested closures. See §3.3 for example definitions of each type.

- $\forall n, \text{natp}(n) \rightarrow \text{power-tail}(n) = \text{power}(n)$, where **power-tail** and **power** calculate powers of 2.
- $\forall n, \text{natp}(n) \rightarrow \text{fib-tail}(n) = \text{fib}(n)$, where **fib-tail** and **fib** calculate fibonacci numbers.
- $\forall x, \text{nat-listp}(x) \rightarrow \text{sort}(\text{sort}(x)) = \text{sort}(x)$, for list-of-natural-numbers predicate **nat-listp** and list-sorting function **sort**.
- $\forall x, \text{true-listp}(x) \rightarrow \text{rev}(\text{rev}(x)) = x$, where **true-listp** ensures that x is a valid singly-linked list structure and **rev** is list reversal.
- $\forall x, \text{true-listp}(x) \rightarrow \text{int}(x, x) = x$, where **int** is the intersection of lists (i.e. a list of elements common to each).

3.3 Auxiliary Lemmas

One consideration when generating conjectures is the difference between theorems, lemmas, corollaries, etc. From a logical point of view, these are all equivalent, and hence most proof assistants do not distinguish between them. However, their *intention* may be different: in a sense, theorems are the interesting results; whilst lemmas are useful results, required for proving the theorems.

Some systems, like Coq, allow users to *label* each statement as being a Theorem, a Lemma, etc. despite their internal representations being the same. This shows us immediately that lemmas outnumber theorems; in the Coq standard library there are over five times as many lemmas as theorems⁵.

We can find a need for auxiliary lemmas, once again, in the context of tail-recursive functions. Consider proving the (pointwise) equality of the following Coq functions, defined for the Peano naturals **Z** and **S**:

```

Inductive Nat : Set := Z : Nat
  | S : Nat -> Nat.

Fixpoint plus      (n m : Nat) := match n with
  | Z   => m
  | S n' => S (plus n' m)
end.

Fixpoint plus_tail (n m : Nat) := match n with
  | Z   => m
  | S n' => plus_tail n' (S m)
end.

```

Both of these functions implement addition, but the **plus.tail** variant is tail-recursive. However, if we want to *prove* that the definitions are (pointwise) equal, we run into difficulties. In particular, when the inductive step requires us

⁵The latest version as of writing is **coq-8.4p16** which, when excluding comments, includes 1492 occurrences of **Theorem** and 7594 of **Lemma** in its **theories/** directory.

to prove $\text{plus } (S\ n)\ m = \text{plus } n\ (S\ m)$ (which seems reasonable), we cannot make this go through using another inductive argument.

Specifically, the *conclusion* of a second inductive hypothesis is exactly the equation we need:

$$\text{IHn}' : (\text{forall } x, \text{plus } n'\ x = \text{plus.tail } n'\ x) \rightarrow \text{plus } (S\ n')\ m = \text{plus } n'\ (S\ m)$$

Yet we cannot provide it with the argument it needs, as our original induction hypothesis is *too specific* (i.e. it has too many S constructors):

$$\text{IHn} : \text{forall } x, \text{plus } (S\ n')\ x = \text{plus.tail } (S\ n')\ x$$

We are forced to abandon the proof, despite such a reasonable-looking intermediate goal.

In fact, if we attempt to prove that goal *separately*, we can use a straightforward argument by induction; even though it is actually *stronger* due to the absence of the IHn assumption. Using this separate result as a lemma, the pointwise equality is proven easily.

3.4 Tests

Since we are working in the domain of Haskell programs, an abundant source of statements are available in the form of *tests*. For manually-written tests, the effort required to write them implies that they must be of some interest to their author. Many forms of test are *not* suitable for our purposes, such as *unit tests* which are always trivially provable by β -reduction; or *integration tests*, which depend on the behaviour of the external environment. One reason to study Haskell is its widespread use of *property checking*, which does give us useful data. Many Haskell property checkers exist, based on random testing (QUICKCHECK [16] and SMARTCHECK [64]), enumeration (SMALLCHECK [72]), observation (LAZY SMALLCHECK [69]) and logic programming (SPARSECHECK [55]).

Thankfully the major differences between these systems are in the way they instantiate test arguments; their representations of properties are largely the same (modulo renaming of functions and types).

Here we consider the 10 most-downloaded packages from HACKAGE (as of 2015-10-30) which have property tests; these are `warp`, `aeson`, `text`, `lens`, `conduit`, `pandoc`, `attoparsec`, `scientific`, `yesod-core` and `blaze-html`.

4 Related Work

4.1 Exploration in Artificial Intelligence

Theorem proving is not the only area of AI to have automation extended from problem *solving* to problem *invention*. Here we consider similar approaches in a variety of domains, and identify techniques which could be re-purposed in the context of theory exploration.

4.1.1 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 in 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 viable approach to the search component of theory exploration.

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.

The evolutionary analogue of theory exploration is to remove the (explicit) fitness function, just like we remove explicit goals to turn the theorem proving task into the theory exploration task. There are two main reasons for studying such purely-exploratory evolutionary systems: *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 the search aspect of 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. [8]).

On the other hand, work on deceptive problems is highly relevant, as it has lead to studying *exploration in general*, and hence provides insight for our narrower domain of theory exploration. Deceptive problems are those where “pursuing the objective may prevent the objective from being reached” [42], 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 to avoiding deception, such as *nicheing methods* [74], alter the output of the fitness function to promote *diversity* and *novelty*. For example, *fitness sharing* promotes diversity by dividing up the fitness of identical or similar solutions, e.g. the result of a fitness function f may be shared by two identical solutions s_1 and s_2 , such that the augmented fitness $f'(s_1) = \frac{f(s_1)}{2}$ and $f'(s_2) = \frac{f(s_2)}{2}$. As always, there are many variations on this theme, such as how to judge similarity (e.g. “genetically” by comparing the solutions themselves, or “phenotypically” by comparing their fitness), but all strive to penalise duplication and hence promote diversity.

Once we augment fitness functions, to a greater or lesser degree, an obvious question arises: what if the augmented function contains nothing of the original fitness? This is the pure exploration scenario we are interested in, which has been found to provide useful “stepping stones”, even in objective-driven domains [42] [32].

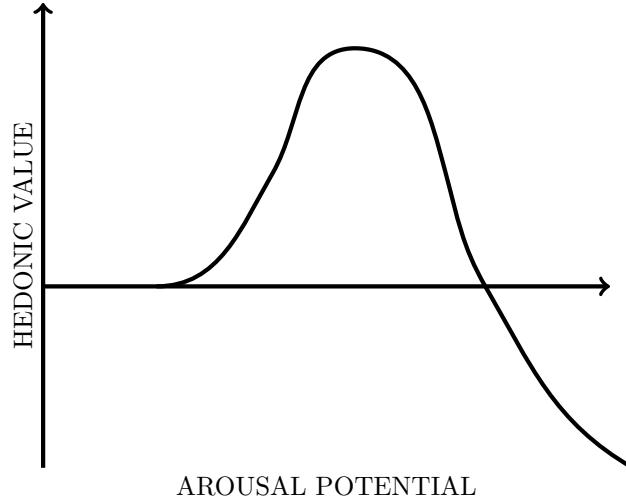


Figure 1: The Wundt curve, reproduced from [9]. The axes “hedonic value” and “arousal potential” are described as covering “reward value... preference or pleasure”, and “all the stimulus properties that tend to raise arousal, including novelty and complexity”, respectively.

4.1.2 Artificial Curiosity

Artificial curiosity (AC) describes active learning systems which are rewarded based on how interesting the input or data they discover is [78], and hence provides a general mechanism for converting goal-driven algorithms into exploration systems. As an unsupervised learning task, AC has no access to labels or meanings associated with this input; the only features it can learn are the structure and relationships inherent in the data. The aim 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 1)⁶, which has been used in psychology to explain human aesthetics and preferences [9].

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

A framework encompassing many interestingness measures, referred to as *implicit rewards* in the reinforcement learning context, is given in [60].

One particularly general measure is *compression progress*: given a com-

⁶In practice, many measures avoid negative values for simplicity, in which cases we replace all negative points on the curve with zero.

pressed 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.

[77]

Two sources of intrinsic reward are proposed in [30] 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 [13]. 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_{KL} of each prediction $P_1 \dots P_m$ from every other prediction:

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

$D(s, a)$ 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).

[36] [45] [46] [47] [68] [71] [75] [77] [76] [80] [82] [48] [52] [59] [61] [78]

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.

4.2 Statistics of Formal Systems

The core problem of assigning “interestingness” to logical formulae is the application of statistical reasoning to the discrete, semantically-rich domain of formal systems. This problem has been tackled from various directions for a variety of reasons; here we summarise those contributions which seem of particular importance for theory exploration.

4.2.1 Relevance

The combinatorial nature of formal systems causes many proof search methods, such as resolution, to have exponential complexity [25]; 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), 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* [50]), 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-occurring 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 [39]. 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

4.2.2 Clustering

4.2.3 Probability of Sentences

The most important property of a logical formula is its truth value. Although we may be able to determine some truth values exactly, e.g. using decision or semi-decision procedures, it may be more efficient to *approximate* truth values. One straightforward extension of truth values is *probabilities*, where we can assign

probability 1 to formulae which are known to be true, 0 to formulae known to be false, and intermediate values to those which we do not yet know.

[33]

4.2.4 Interestingness in Concept Formation

[53] [63] [88] [20] [21] [19] [43] [54] [15] [34] [81] [19]

4.2.5 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.

4.2.5.1 Feature Extraction *Feature extraction* is a common pre-processing step for machine learning (ML). Rather than feeding “raw” data straight into our ML algorithm, we only learn a sample of *relevant* details, known as *features*. This has two benefits:

- *Feature vectors* (ordered sets of features) are chosen to be more compact than the data they’re extracted from: feature extraction is *lossy compression*. This reduces the size of the ML problem, improving efficiency (e.g. running time).
- We avoid learning irrelevant details such as the encoding system used, improving *data* efficiency (the number of samples required to spot a pattern).

Another benefit of feature extraction is to *normalise* the input data to a fixed-size representation. Many ML algorithms only work with fixed-size inputs; for example, the popular *backpropagation* [73] algorithm works on models with *fixed* topology (e.g. *artificial neural networks* with fixed connections between nodes). This requires some form of pre-processing in domains where the size of each input is not known, may vary or may even be unbounded.

For example, in the case of *online* learning we must make predictions/decisions before seeing all of the inputs. Unbounded input appears in domains such as programming and theorem proving, where individual term may be trees of unbounded depth. In these situations we need a mapping from arbitrary inputs to a fixed representation which is amenable to learning.

As an example, say we want to learn relationships between the following program fragments:

```
data Maybe a = Nothing | Just a
```

```
data Either a b = Left a | Right b
```

We might hope our algorithm discovers relationships like:

- Both are valid Haskell code.
- Both describe datatypes.
- Both datatypes have two constructors.
- **Either** is a generalisation of **Maybe** (we can define **Maybe a = Either () a** and **Nothing = Left ()**).
- There is a symmetry in **Either**: **Either a b** is equivalent to **Either b a** if we swap occurrences of **Left** and **Right**.
- It is trivial to satisfy **Maybe** (using **Nothing**).
- It is not trivial to satisfy **Either**; we require an **a** or a **b**.

However, this is too optimistic. Without our domain-knowledge of Haskell, an ML algorithm cannot impose any structure on these fragments, and will treat them as strings of bits. Our high-level hopes are obscured by low-level details: the desirable patterns of Haskell types are mixed with undesirable patterns of ASCII bytes, of letter frequency in English words, and so on.

In theory we could throw more computing resources and data at a problem, but available hardware and corpora are always limited. Instead, feature extraction lets us narrow the ML problem to what we, with our domain knowledge, consider important.

There is no *fundamental* difference between raw representations and features: the identity function is a valid feature extractor. Likewise, there is no crisp distinction between feature extraction and machine learning: a sufficiently-powerful learner doesn't require feature extraction, and a sufficiently-powerful feature extractor doesn't require any learning! ⁷

Rather, the terms are distinguished for purely *practical* reasons: by separating feature extraction from learning, we can distinguish straightforward, fast data transformation (feature extraction) from complex, slow statistical analysis (learning). This allows for modularity, separation of concerns, and in particular allows “off-the-shelf” ML to be re-used across a variety of different domains.

Even if we have no domain knowledge, we can still use a feature extraction phase to improve efficiency: first we learn a compact representation for our data, for example using *autoencoding*; then we use that encoder as a feature extractor for our main learning task. This stacking of one learning algorithm on top of another, especially with greedy learning of each layer, has led to the recent trend of *deep learning*.

⁷Consider a classification problem, to assign a label $l \in L$ to each input. If we only extract a single feature $f \in L$, we have solved the classification problem without using a separate learning step.

4.2.5.2 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 [27], which limits itself to trees with at most 10 levels and 10 elements per level; each tree is converted to a 30×10 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.

4.2.5.3 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).

4.2.5.4 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 [87]. 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 [31]).

The application of *kernel methods* to structured information is discussed in [22], where the input data (including sequences, trees and graphs) are represented using *generative models*, such as hidden Markov models, of a fixed size.

[22] [62] [5] [65] [24] [41] [67] [90]

5 Contributions

5.1 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 $t :: \text{Tree}$ 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 $w \times d$, 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 [90] we have investigated the use of *circular convolution* (cc) as our combining function. Hence, to reduce $t :: \text{Tree}$ to a single feature vector, we can use $\text{reduceC } t$ where:

$$\begin{aligned} \text{reduceC (Leaf } fv) &= fv \\ \text{reduceC (Branch } fv \mid r) &= cc \, fv \, (cc \, (\text{reduceC } l) \, (\text{reduceC } r)) \end{aligned}$$

Circular convolution has the following desirable properties:

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

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

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 $(FV, FV) \rightarrow FV$ 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* [65].

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.

5.1.1 Extracting Features from XML

This method of folding with circular convolution has been implemented in the Haskell program TREE FEATURES⁸. The feature is then:

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

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

⁸Available 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

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.

5.1.2 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.

5.2 nix-eval

5.3 ASTPlugin

The Glasgow Haskell Compiler provides a library interface to its operation, which we can use to parse Haskell code into tree structures. It also provides 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.

5.4 MLSpec

5.5 ML4HS

We identify the following potential improvements for existing TE systems such as HIPSPEC:

Term generation: Enumerating all type-correct terms is a brute-force solution to this question. Scalable alternatives to brute-force algorithms are a well-studied area of Artificial Intelligence and Machine Learning. In particular, heuristic search algorithms like those surveyed in [11] could be used. We could also use Machine Learning methods to identify some sub-set of a given theory, to prioritise over the rest.

Interestingness Various alternative interestingness criteria have been proposed, for example those surveyed in [23]. Augmenting or replacing the criteria

may be useful, for example to distinguish useful relationships from incidental coincidences; or to prevent surprising, insightful equations from being discarded because they can be simplified.

We are implementing a system called ML4HS to investigate these ideas. Its current form is a pre-processor for QUICKSPEC for prioritising theory elements. Inspired by the use of premise selection [40] to reduce the search space in ATP, we select sub-sets of the given theory to explore, chosen to try and keep together those expressions which combine in interesting ways, and to separate those which combine in uninteresting ways.

We hypothesise that similarity-based clustering of expressions, inspired by that of ML4PG [38] and related work in ACL2 [29], is an effective method for performing this separation. Future experiments will test this by comparing the throughput of QUICKSPEC with and without the ML4HS pre-processor.

6 Future Work

7 Conclusion

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