Refinement type contracts for verification of scientific investigative software

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Abstract. Our scientific knowledge is increasingly built on software output. User code which defines data analysis pipelines and computational models is essential for research in the natural and social sciences, but little is known about how to ensure its correctness. The structure of this code and the development process used to build it limit the utility of traditional testing methodology. Formal methods for software verification have seen great success in ensuring code correctness but generally require more specialized training, development time, and funding than is available in the natural and social sciences. Here, we present a Python library which uses lightweight formal methods to provide correctness guarantees without the need for specialized knowledge or substantial time investment. Our package provides runtime verification of function entry and exit condition contracts using refinement types. It allows checking hyper-properties within contracts and offers automated test case generation to supplement online checking. We co-developed our tool with a medium-sized (≈3000 LOC) software package which simulates decision-making in cognitive neuroscience. In addition to helping us locate trivial bugs earlier on in the development cycle, our tool was able to locate four bugs which may have been difficult to find using traditional testing methods. It was also able to find bugs in user code which did not contain contracts or refinement type annotations. This demonstrates how formal methods can be used to verify the correctness of scientific software which is difficult to test with mainstream approaches.

Keywords: formal methods · scientific software · contracts · refinement types · python · runtime verification.

1 Introduction

Over the last several decades, software engineering has made great strides in developing tools and processes for verifying the correctness of computer software. Although verification has been strikingly successful across many different domains, it has not been widely applied to scientific software. It has been estimated that 5%-100% of scientific software output is incorrect due to undetected software bugs [44], and this is evident from the many retractions caused by undetected bugs[1]. Some of these retractions were covered in depth by the popular

1 See [http://retractionwatch.com/](http://retractionwatch.com/)
press. In one case, a researcher discovered that the results defining his career were built on a software bug, forcing him to retract five of his most important papers from top journals [33]. In another case, a software bug reversed the results of highly influential economics research which was widely cited in public policy decisions [23]. Section 2 will provide concrete examples which illustrate common sources of such bugs.

One ubiquitous class of scientific software has received little to no attention from the verification community: this software is user code which is characterized by (a) small amounts of code (usually 50-500 LOC) (b) written by domain experts with little to no formal training in software engineering [19,8,39], which is (c) run a limited number of times, (d) has specifications that change unpredictably on a daily or hourly basis, (e) is used almost exclusively by the original developer, and (f) has no testing oracle because the output of the software is the object of investigation [21,29,44]. We refer to this class of software as “investigative software”. Investigative software is written on a daily basis by countless researchers across the natural and social sciences. Some common examples of investigative software include: scripts to load experimental data and perform statistical tests using statistical libraries; simulations of a computational model; a pipeline which performs complicated preprocessing operations on input data; or a script used internally to make business decisions. This paper presents a tool which is used to verify investigative software.

Testing and verifying correctness of investigative software is difficult due to many technical and cultural factors including unclean data, the lack of a testing oracle, and the insufficiency of standard testing procedures for the structure and goals of scientific programs [30,25,26,27,28,40]. There already exist methods in the scientific community for checking program correctness, but they have serious limitations which limit their utility as discussed in Section 7; as a result, investigative software is most commonly validated by determining whether the program’s output matches the expectations of the scientist, posing a fundamental violation of the scientific method [40]. A more convenient and effective method for ensuring the quality of scientific software is needed.

Formal methods are able to check the correctness of investigative software. However, state of the art formal verification tools are time-consuming to implement and require substantial formal methods expertise, which make their use impractical for investigative software. A survey estimated that scientists spend about 30% of their time writing software [19], so the need to formally verify this code is a substantial hurdle to productivity.

By contrast, runtime verification is easy to use and especially well-suited to investigative software. It requires little training to use, yet is able to achieve many of the same goals; because investigative software is usually developed by its sole user, it doesn’t matter whether bugs are caught during development or detected at runtime through verification condition violations. This reflects the fact that investigative software development often cannot be meaningfully separated from data analysis [34,25,31,40]. Researchers need access to lightweight
formal methods to improve the correctness of their software without slowing down the research process.

We created Paranoid Scientist\(^2\), a Python library for verifying the correctness of investigative software. Paranoid Scientist employs runtime verification to check software correctness. Developers specify function behavior through entry and exit conditions, thereby creating function contracts which must be satisfied by each function execution \(^{2,20}\). Contracts are specified in two parts. First, each function argument and the return value are specified modularly using refinement types \(^{14,46}\), which are types defined by predicates. Second, additional constraints such as a dependence of the return type on the function arguments or the function argument types on each other are specified using predicates written in pure Python. These constraints may also depend on previous calls to the function in order to check hyperproperties. In addition to runtime checking, Paranoid Scientist may further use the refinement type contracts to automatically generate test cases. Critically, Paranoid Scientist uses simple syntax and is intuitive to those without a background in formal methods or software engineering. We ran our tool on real-world investigative software and found that it was able to catch four undetected bugs while imposing a 1.05–6.41 factor performance penalty.

2 Motivating examples

We provide two motivating examples from real-world investigative software written for research in the biomedical sciences.

Incorrect function usage Figure 1a shows an example bug in a function designed to find the reverse complement of a DNA sequence. Briefly, DNA is the primary medium for long-term information storage in biological organisms. Each strand is composed of long sequences of four “base” molecules—adenine (A), guanine (G), cytosine (C), and thymine (T). For chemical stability, each strand of DNA within an organism is usually bound to a “reverse complement” strand whereby the A and T bases and the G and C bases are swapped and the resulting sequence is reversed. By contrast, RNA is a biological medium for short-term information storage. It shares a nearly identical structure with DNA, but replaces T with uracil (U). Consequently, when forming the RNA reverse complement, A is swapped with U instead of T.

The function \texttt{complement\_sequence} in Figure 1a uses a simple mechanism to compute the reverse complement DNA sequence. It accepts a list of characters and, using Python’s equivalent of the Unix program “\texttt{tr}”, it converts all A to T, G to C, C to G, and T to A, and then reverses the result. While this function behaves as intended, an erroneous usage of the function occurs when the user tries to find the reverse complement of an RNA sequence instead of a DNA sequence. The function accepts the valid RNA sequence \texttt{UCG} and returns another valid RNA sequence \texttt{CGU} without error. However, \texttt{CGU} is not the reverse complement of

\(^{2}\) https://github.com/mwshinn/paranoidscientist
def complement_sequence(seq):
    c_str = ''.join(seq).translate(str.maketrans('AGCT', 'TCGA'))
    return list(reversed(c_str))

complement_sequence(['A', 'T', 'C'])
complement_sequence(['U', 'C', 'G'])

Fig. 1: Two examples illustrate real-world bugs in investigative software. (a) A function designed to process DNA sequences is invoked with an RNA sequence. Due to their similarity, a valid but incorrect output is returned for the RNA sequence. (b) NaN values can be silently propagated. This code constructs an undirected graph weighted by transformed pairwise correlations of brain scan timeseries. The fisher_transform function is accidentally applied twice, the second execution of which generates a matrix with some NaN values which are silently ignored in the matrix_to_graph function.

UCG, because the U should be replaced with an A. The complement_sequence function is only designed to operate on DNA sequences, and thus cannot properly deal with the RNA base U.

Paranoid Scientist is able to ensure correctness in this example. An annotated version of the complement_sequence function is shown in Figure 2a. Most importantly for this example, the @accepts decorator checks that the argument value is a list consisting only of values A, G, C, and T. This means that passing an RNA sequence to the function in Figure 1a will raise an error, because the “U” element in the list is invalid for DNA. Even if entry conditions were not specified, the “U” would have been caught as an invalid output type by the return type specification in the @returns decorator, and by the exit condition in the @ensures decorator which specifies that all values of the input must be different than the corresponding values of the reversed output. These properties are checked at runtime to ensure the function is receiving correct input and producing correct output.

NaN propagation Another example bug is shown in Figure 1b, which is a condensed version of a bug from real-world investigative software. This code is the final step in a pipeline which converts a functional magnetic resonance imaging (fMRI) scan—a type of brain scan which allows researchers to look at brain activity over time—to an undirected graph where edges represent strong correla-
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```python
def complement_sequence(seq):
    ...
```

```python
def fisher_transform(corr_values):
    ...
```

(a) Annotations for Figure 1a

(b) Annotations for Figure 1b

Fig. 2: Two examples of Paranoid Scientist annotations which could detect the bugs in Figure 1a and 1b. (a) Ensure that the `complement_sequence` function accepts and returns DNA sequences. (b) Ensure that the `fisher_transform` function only receives values for which it is defined, and that it always returns a number (i.e. not NaN or ±inf).

In brain activity [4], first, several computationally-intensive preprocessing steps are applied to the timeseries, and then the pairwise Pearson correlation of each region is computed. Pearson correlation is a value from -1 to 1 inclusive, which is converted to a more statistically-informative value from negative infinity to infinity using the Fisher z-transform, or equivalently hyperbolic arctangent. This is then saved to a file so that the computationally intensive steps do not need to be repeated.

After saving, the timeseries can be reloaded and turned into an undirected graph. However, before doing so, the `fisher_transform` function is erroneously applied a second time. The second time it is called, the inputs hold values from negative infinity to infinity. This is outside of the domain of the hyperbolic arctangent function, causing it to return NaN for inputs less than -1 or greater than 1. In practice, this gives reasonable values for small- and medium-valued correlations but NaN for large correlations. These NaN values are masked by the function `matrix_to_graph`, returning a graph which does not show evidence of the NaN values; this creates a graph which appears to be correct for all but the largest correlations. This bug therefore created subtle changes in the resulting graph topology which were not noticed immediately, causing several weeks of work analyzing the resulting graphs to be lost.

Paranoid Scientist is able to detect this bug. Figure 2b shows annotations for the `fisher_transform` function. This function takes any N-dimensional array (NDArray) with values ranging from -1 to 1, and returns an N-dimensional array of the same shape with elements which are numbers. NaN is not a valid number. These annotations would have been sufficient to catch the bug in Figure 1b. Alternatively, annotations which specified the valid input of `matrix_to_graph` would have also been able to detect this bug.

If either of these two bugs had appeared in software which had an oracle, there is a high probability that the difference in behavior would manifest as an observable bug and the behavior could be corrected [29]. Investigative software is written because the result is unknown, so in these cases the bugs may never have been found.
3 Package summary

3.1 Refinement types

Function entry and exit conditions are specified in part by refinement types. In our tool, refinement types are defined by a predicate which checks whether an input is an element of the type. Predicates are constructed by Python functions using purely Python code, and thus may reach arbitrary levels of complexity without depending on a domain specific language. This allows types to be defined in terms of their scientific purpose and conceptual properties instead of as datatypes [46]. These refinement types are akin to what one would write when documenting the function. For example, one type defined by default is “Number”, which can be a float or an int but not NaN or ±inf. Types can also represent more complex properties. For example, a discrete probability distribution is a list with non-negative elements which sum to 1, and a correlation matrix is a symmetric positive semidefinite matrix with 1 on the diagonal. A list of all types included by default is included in the Appendix. Any class can be used in place of a type by checking whether the passed value is a subclass of the given class. Alternatively, classes can define a method to determine whether the passed value is an instance of the class, described in further detail in Section 3.3.

3.2 Entry and exit conditions

In addition to refinement types, additional entry and exit conditions may be specified for conditions involving multiple function arguments or involving function arguments and the return value. For example, there may be a constraint that the first argument is greater than or equal to the second argument, or that the function returns a matrix with the number of rows and columns specified by the input arguments. Conditions are specified as a string which is evaluated as Python code.

Function properties may depend on more than a single execution of the function. For example, function concavity and function monotonicity are hyperproperties which cannot be determined at runtime when considering a single function execution. Paranoid Scientist saves in memory a list of arguments and return values from previous function executions. All future function executions are compared against these past values. For functions which are executed many times, a naive implementation would cause serious performance and memory penalties, limiting the practicality of this feature. We address this problem by saving only a subset of function calls and using reservoir sampling [48] to test against a uniform distribution across all function calls; as a result, verification of hyperproperties is not performed across all previous calls but rather checked across a sample of previous calls which is uniformly-distributed across time. An example of one such hyperproperty is shown in Figure 3.
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Fig. 3: Example of a hyperproperty. For any two executions of this function, Paranoid Scientist will check that the monotonicity hyperproperty is satisfied.

3.3 Syntax

Refinement types for function arguments and return values are specified using the @accepts and @returns function decorators, respectively. Further entry and exit conditions are passed as strings of Python code to the @requires and @ensures function decorators, respectively. The strings are evaluated using a namespace which includes the function arguments and additional user-specified libraries. In @ensures, the special value return represents the return value of the function. For testing hyperproperties, function arguments and return values from previous executions can be accessed by appending one or more backtick characters as a suffix, a notation which is reminiscent of the “prime” symbol from mathematics. Additionally, syntactic sugar is available for the two common idioms “implies” with the --> syntax and “if and only if” with the <-> syntax.

In addition to the default types, refinement types may be defined manually. Types are classes which define two methods: one to test values for adherence to the type, and a second to generate values of the type for use in automated testing, as described below. The type definition may optionally accept arguments to specify parameterizable behavior or generics. Any existing class can also be used as a type by using the class name in place of a refinement type. In these cases, Paranoid Scientist only tests whether the element is an instance of the class, where adherence to the Liskov substitution principle is assumed by default, i.e. subclasses are also considered to be elements of their parent class. For more precise control over the checking, class methods may be defined analogous to the methods for testing and generating values in stand-alone refinement types, allowing a single class to serve both as a normal class and also as a refinement type.

3.4 Automated testing

The use of entry and exit conditions for each function makes it possible to perform unit tests automatically. A stand-alone command line utility takes the program to be checked as input and individually tests each function in the program with values generated using a specialized method from the refinement type specifications, similar to fuzz testing [12]. These generated values are passed as arguments to each function as long as the values satisfy the function’s entry conditions. Because investigative software very seldom includes tests, this increases robustness.
Table 1: Performance benchmarks. Runtime for each example program is shown with standard error of the mean over 10 runs.

|                   | design | versatility | pyddm_sim | pyddm_fit |
|-------------------|--------|-------------|-----------|-----------|
| Total LOC         | 162    | 86          | 5         | 20        |
| Program LOC       | 117    | 68          | 5         | 20        |
| Annotation LOC    | 45     | 18          | (user code) | (user code) |
| % Code annotations| 28%    | 26%         | 0%        | 0%        |
| Runtime w/ checking (s)| 8.45 ± 0.052 | 29.047 ± 0.158 | 13.685 ± 0.057 | 4.726 ± 0.160 |
| Runtime w/o checking (s)| 3.239 ± 0.022 | 27.606 ± 0.205 | 2.136 ± 0.013 | 3.066 ± 0.121 |
| Slowdown factor   | 2.61   | 1.05        | 6.41      | 1.54      |

Not all functions can be tested. Those with unspecified types, strict entry conditions, or arguments which cannot be automatically generated will not produce any test cases. Likewise, some tests run for a very long time under certain parameterizations; these are killed after some designated time duration to balance correctness with the practical constraints of testing. Paranoid Scientist will report to the user a list of the functions which could not be tested so that these may be targeted for further testing.

More detailed information about syntax and automated testing is available in the package documentation.

4 Performance evaluation

We evaluate the runtime performance of Paranoid Scientist on several examples programs drawn from investigative software in cognitive neuroscience.

- **Design matrix construction (design)** Construct a design matrix for a generalized linear model, similar to the analysis performed in [35].
- **Nodal versatility (versatility)** Compute the versatility [42] of a node in an undirected graph with respect to a community detection algorithm.
- **Decision-making simulation (pyddm_sim)** Simulate decision-making using the PyDDM software package (see Section 5).
- **Decision-making fitting (pyddm_fit)** Fit a decision-making model to simulated data using the PyDDM software package (see Section 5).

Performance benchmarks are shown in Table 1. Overall, annotations comprised between 25-30% of the lines of code. There is a performance penalty for runtime verification, and this penalty varies depending on the details of the code. This penalty falls within the ranges suggested for “deliverable” (a 3x slowdown) or “usable” (10x slowdown or less) in runtime checks [45].

These examples were derived from real-world investigative software. Notably, a previously undetected bug was found in the design example when Paranoid Scientist annotations were added to it, which caused incorrect binning of data before performing the regression analysis.
5 Case study

We used our tool while developing PyDDM, a decision-making simulator for cognitive neuroscience. PyDDM’s development was initially intended for a specific series of studies and was later released to other research groups [15]. Overall, Paranoid Scientist annotations comprised about 10% of the codebase. Over 95% of these annotations require refinement types which cannot be checked using existing static type checkers for Python. Hyperproperties were specified for less than 5% of function exit conditions.

We briefly describe the motivation for PyDDM. PyDDM aids in the study of a simple form of decision-making whereby two options are presented and the subject must choose one of the two based on either preference or matching a given stimulus. This type of decision-making is often studied using the drift-diffusion model (DDM), which posits that all decisions consist of some underlying evidence signal plus noise in continuous time [38]. The process of making a decision relies on integrating evidence for each option over time and coming to the final decision when the total integrated evidence surpasses some confidence criterion. Decision-making is usually studied for simple decisions over a short duration of time (5 sec), such as for determining whether a sock is black or dark blue, but the model can also be used for decisions which may span days or weeks, such as deciding between two job offers. In either case, there is a trade-off between the time it takes to make the decision and the accuracy expected.

The DDM represents evidence integration as a diffusion process governed by the first passage time of a stochastic differential equation across a boundary. Analytical solutions for the DDM are fast to compute, but only specific versions of the model can be solved analytically. Recent experiments have found that humans and animals exhibit behavior which differs from these specific versions of the model. In order to explain experimental data, it is necessary to use a more general version of the model which can only be solved numerically. PyDDM provides a consistent interface to a collection of analytical and numerical algorithms for solving the generalized DDM, selecting the best routine for each model.

As a result, PyDDM contains a mix of optimized routines for finding solutions to stochastic differential equations, and a set of object-oriented interfaces to make these routines convenient to use. This includes predefined models for the most common use cases. Consequently, PyDDM must be used in conjunction with user code written by neuroscience researchers who may have limited experience in software engineering. Thus, the goals of verification are two-fold: detecting errors in PyDDM itself, and detecting errors in PyDDM user code.

5.1 Detecting errors in PyDDM

We found four non-trivial bugs in PyDDM using Paranoid Scientist. Briefly, the bugs were:

3 https://github.com/mwshinn/PyDDM
1. Under certain circumstances, a small function which was assumed to return a positive number would return a negative number due to a typo in a mathematical equation. This was caught by a return type of “Positive”.

2. An algorithm assumed that the output of a previous step in the processing pipeline yielded a vector with 0 as the first element. It was intuitive that this should be the case. When the numerical algorithm was upgraded, this no longer held true. Only one distant branch in the pipeline relied on this value being zero. This was caught by a precondition specifying the first element of the array should be 0.

3. When a model of a particular form was fit to data, a discretization approximation in a non-central portion of the code would exploit the limited numerical resolution of the simulation in order to select unnatural parameters which in turn artificially inflated the model’s performance metrics. This was caught by a postcondition which checked that the distribution would integrate to 1.

4. Particular inputs caused numerical instabilities in one of the three simulation methods and made the probability distribution contain values slightly less than 0. This was caught by a precondition on a different function which required all elements of the input array to be greater than 0.

Bugs (1) and (2) would have been very difficult to detect without our tool, and detecting bug (3) would have required manually examining a large amount of intermediate output. These three bugs would have slightly impacted scientific results. Bug (4) would have likely been noticed eventually but would have caused a substantial time investment to locate. In addition to these bugs, Paranoid Scientist was able to detect an internal inconsistency in how data were stored. Though this did not manifest in a bug which affected results, it had the potential to do so in the future.

5.2 Detecting errors using traditional methodology

In addition to Paranoid Scientist annotations, unit tests and manual code review were used to catch bugs in PyDDM. One non-trivial bug was found in unit testing which was not detected by Paranoid Scientist, but this bug did not impact results:

1. When the core simulator’s representation of a probability distribution was extended to include support for storing the distribution of incomplete trials, this unexpectedly modified the behavior of a distant piece of the code which utilized that representation.

Additionally, two non-trivial bugs were detected through code review which neither Paranoid Scientist nor unit/integration tests were able to catch; these bugs also did not impact results:

1. When constructing a diffusion matrix as a part of the core simulation routine, certain rare but important cases utilized the previous timestep instead the next timestep.
2. A simulation algorithm is automatically chosen for each model, but this choice was suboptimal for a small number of models.

5.3 Detecting errors in user code

In addition to PyDDM’s core library code, a key feature is its extensibility with user code to define new models. Due to the complexity of models which can be defined by users, it is important to catch errors in user code even if the users do not use Paranoid Scientist annotations.

Paranoid Scientist was able to find three bugs in user code, even though this code did not have Paranoid Scientist annotations. All three of these would have impacted results:

1. Two subjects completed an experimental task with different task parameters, but parameters were mixed because the expression \( \text{if subject == 1} \) should have been \( \text{if subject != 1} \). This caused a parameterization which was valid on its own but not within the context of the data. This was caught by a precondition which checked that one parameter was less than or equal to all elements of a data array.

2. A user-defined function to generate discrete probability distributions sometimes produced an invalid distribution. This was caught by a precondition checking that the distribution summed to 1.

3. Boundaries were initialized randomly according to a normal distribution. However, sometimes these bounds would be erroneously initialized such that some mass of the initial probability distribution had already crossed the bounds. This was caught by a precondition which checked that two input vectors were the same size.

6 Limitations

Runtime checking imposes penalties on the program’s speed. Paranoid Scientist has not been optimized for speed, though such optimization is possible in the future. Previous work has demonstrated improved performance of runtime checks through a client–server architecture [10] and through optional contracts [11]. Performance could also be improved by producing a certificate during runtime which can be checked after execution.

Paranoid Scientist is compatible with all Python features and does not require the programmer to limit herself to a Python subset or to use a wrapper of the Python executable. Nevertheless, some less-commonly used Python features may cause problems if incorporated into contracts due to the present implementation of runtime checking, especially if these features are stateful. For example, Python objects are allowed to change their value when accessed, but this violates the assumptions of runtime checking. Likewise, contracts cannot yet be specified for generators. If these features are needed in contracts, Paranoid Scientist includes the Unchecked type as an alternative.
During runtime, Paranoid Scientist is able to implicitly deal with side effects relevant to the results of the computation such as modifications to global state and file IO. However, automated tests are unable to deal with these side effects. Paranoid Scientist does not have an explicit model of these or other side effects such as exceptions and printing, because a clear specification of these is seldom critical for investigative software.

Python’s syntax for type annotations provides a convenient way to specify types. Paranoid Scientist uses function decorators instead of type annotations. Type annotations would be suitable for the @accepts and @returns decorators, but not for the @requires or @ensures decorators, so using decorators for all of these improves syntax consistency. The use of decorators allows type annotations to be used for other purposes in the same codebase, and may avoid confusion among less-experienced Python programmers who are not used to this new syntax, or among users who run older versions of Python.

7 Related work

Formal methods for scientific software The present focus on investigative software differs from previous work on verifying scientific software, which focuses on floating point operations or high performance computing. These tools are effective for specific types of scientific software, but the methodology they impose does not reflect the environment in which most investigative software is written and used. Besides formal methods, prior work on testing scientific software does not focus on investigative software; instead, it focuses on large or collaborative software projects, software written by seasoned software engineers instead of researchers with limited formal training, software without an oracle, or computationally- or numerically-intensive software.

Testing scientific software Several recognized methods exist for software testing in the scientific community, but these methods have serious limitations. One method involves rewriting a piece of software one or more times by independent parties and comparing the output for identical input. In practice this is not feasible for most investigative software, due to the fact that it is written by a single individual for a limited number of executions. Another method is running the software with simplified parameters or artificial data for which the result is known. This leaves the most scientifically important pieces of the code untested, and it is often difficult to determine equivalence of the software’s output with the known result due to stochasticity or floating point arithmetic. Meta-morphic testing has been proposed as an alternative means of testing software without an oracle, which involves testing specific properties which are required to hold. This requires a deep knowledge of testing methodology and a code structure which facilitates such tests.

4 [https://www.python.org/dev/peps/pep-0484/]
Python type systems In recent years there has been a proliferation of static type checkers within the Python ecosystem, starting with MyPy \[^{5}\] and continued by Facebook's Pyre \[^{6}\], Google's PyType \[^{7}\], and Microsoft's PyRight \[^{8}\]. This has been further advanced by PEP 484 \[^{9}\] which standardized a syntax for type annotations for functions in the Python language. These type checkers introduce neither overhead nor speedups, as the types are checked before and not during runtime. Thus, the type information is not enforced during program execution.

Reticulated Python \[^{10}\] includes runtime checks for annotated types using three different methods. The two bugs described in \[^{11}\] which were caught using Reticulated Python would have occurred as exceptions without runtime checks; with the present work, we are more interested in bugs which might have otherwise gone undetected. One of Reticulated Python’s modes of operation can insert undetected bugs into the code by not preserving object identity, demonstrating the different objectives between Reticulated Python and the present work. Additional packages for runtime checking of static data types in Python, such as the “enforce” \[^{12}\] or “typeguard” \[^{13}\] packages, share many similarities to the “transient” method in Reticulated Python.

Python contracts libraries While contracts were first conceived for Python in the language’s infancy \[^{14}\], contracts are still rare in Python code. The most popular contract library for Python is “PyContracts” \[^{15}\] which embeds a domain specific language into Python for specifying properties that each argument must satisfy. It is difficult to specify complex properties or to create properties which rely on more than one argument, such as “argument 1 is greater than argument 2”. PyBlame \[^{16}\] provides a sophisticated contract library for Python which integrates with the debugger, but a detailed comparison could not be performed due to the lack of availability of the PyBlame source code. Data validation libraries, such as “cerberus” \[^{17}\] and “voluptuous” \[^{18}\] ensure that datasets satisfy particular conditions, and thus may be used in conjunction with Paranoid Scientist.

Nagini is a package which provides full static verification for a Python subset \[^{19}\]. Python code is converted to an intermediate language and conditions are specified using contracts. In addition to arbitrary assertions, it can reason about exceptions, memory safety, data-race conditions, and input–output. However, approximately half of the lines of code must be devoted to the specification, and it has difficulty inferring properties about non-Python code such as C libraries.

\[^{5}\] http://mypy-lang.org/
\[^{6}\] https://pyre-check.org/
\[^{7}\] https://google.github.io/pytype/
\[^{8}\] https://github.com/Microsoft/pyright
\[^{9}\] https://www.python.org/dev/peps/pep-0484/
\[^{10}\] https://github.com/RussBaz/enforce/
\[^{11}\] https://github.com/agronholm/typeguard
\[^{12}\] https://andreacensi.github.io/contracts/
\[^{13}\] https://docs.python-cerberus.org/en/stable/
\[^{14}\] https://github.com/alecthomas/voluptuous
8 Conclusions and future directions

It is difficult to overestimate the importance of investigative software in scientific research, but few studies have examined effective techniques for ensuring its correctness. Paranoid Scientist uses lightweight formal methods to provide correctness guarantees about this difficult-to-test class of software. It does so through a combination of contracts and refinement types in a way which is easy to use for those without explicit training in formal methods. We demonstrated that Paranoid Scientist can be used to find bugs in scientific software which would have impacted results and would have been otherwise difficult to detect.

Investigative software is built in an environment which poses two unique challenges for Hoare-style verification and static checking of preconditions and postconditions. First, the verification technique must be usable by scientists with little to no training in computer science. The state of the art techniques require a deep knowledge of formal methods to use them effectively \cite{13}. Second, the amount of time spent verifying the software must be small compared to the amount of time spent writing the code to be verified. Current techniques are time consuming to implement. By contrast, our tool requires approximately as much time to implement as does writing function documentation.

Technical constraints of investigative software raise further challenges for formal methods. Investigative software in Python relies heavily on non-Python code such as C libraries and integrated shell commands, and thus static verification would require scaffolding for usability in practice. This scaffolding mandates more effort for verification and strong familiarity of the user with formal methods, exacerbating the previously discussed environmental challenges. Additionally, techniques such as type inference are conceptually incompatible with the present approach because the types in Paranoid Scientist often depend on the purpose of the code; for example, it may be “valid” to accept a probability less than 0 but this does not make sense on a scientific level. A gradual static verification approach, analogous to gradual typing \cite{43}, may be useful.

Lightweight formal methods may also be applied to investigative software in other programming languages. The present work targets Python due to its ubiquity in investigative software and powerful metaprogramming capabilities to simplify implementation. Besides Python, common languages for investigative software include Matlab, Julia, and R. While the bug shown in Figure 1b may not have occurred in other languages, different programming languages have different advantages and disadvantages for the correctness of investigative software. For example, Matlab by default defines the constants $i$ and $j$ to be $\sqrt{-1}$, but allows these to be assigned other values by users. As a result, mistaken variable initialization or names can cause undetected bugs. Additionally, unexpected files saved to locations in Matlab’s \texttt{PATH} can cause erroneous versions of scripts or data to be loaded, or even cause built-in functions to change their behavior. An implementation of lightweight formal methods as described here would be able to catch these and other bugs in Matlab.

It is critical to verify the correctness of investigative software, but technical and cultural constraints limit the effectiveness of conventional techniques.
Lightweight formal methods as implemented in Paranoid Scientist provide a convenient and effective way to check the correctness of investigative software.

**Acknowledgments**

Thank you to Ruzica Piskac and Anastasia Ershova for a critical review of the manuscript; Clarence Lehman, Daeyeol Lee, and John Murray for helpful discussions; Michael Scudder for PyDDM code reviews; and Norman Lam for PyDDM development and code reviews. Funding was provided by the Gruber Foundation.

**Appendix: Default types**

### Numerical

- **Numeric**: A floating point or integer
- **ExtendedReal**: A floating point or integer, excluding NaN
- **Number**: A floating point or integer, excluding NaN and ±inf
- **Integer**: An integer
- **Natural0**: An integer greater than or equal to zero
- **Natural1**: An integer greater than zero
- **Range**: A number with a value between two specified numbers, inclusive
- **RangeClosedOpen**: A number with a value between two specified numbers, inclusive on the bottom and exclusive on the top
- **RangeOpenClosed**: A number with a value between two specified numbers, exclusive on the bottom and inclusive on the top
- **RangeOpen**: A number with a value between two specified numbers, exclusive
- **Positive0**: A number greater than or equal to zero
- **Positive**: A number greater than zero
- **NDArray**: A Numpy ndarray, optionally with a given dimensionality or elements which satisfy a given type

### Strings

- **String**: A Python string
- **Identifier**: A non-empty alphanumeric string with underscores and hyphens
- **Alphanumeric**: A non-empty alphanumeric string
- **Latin**: A non-empty string with Latin characters only

### Collections

- **Tuple**: A Python tuple, with elements which satisfy given types
- **List**: A Python list, with elements which satisfy a given type
- **Dict**: A Python dictionary, keys and values which satisfy given types
- **Set**: A Python set, with elements which satisfy a given type
- **ParametersDict**: A dictionary which may include only a subset of keys, with values which satisfy given types

### Logical types

- **And**: Logical AND of two or more types
- **Or**: Logical OR of two or more types
- **Not**: Logical NOT of a type

### Special types

- **Boolean**: Either True or False
- **Function**: A Python function
- **Constant**: A single specified value is accepted
- **Nothing**: Only None, equivalent to Constant(None)
- **Unchecked**: Any value (always succeeds)
- **Void**: No value is accepted (always fails)
- **Maybe**: Either a value of the specified type or else None
- **Self**: The self argument to a method
- **PositionalArguments**: Optional positional arguments to functions
- **KeywordArguments**: Optional keyword arguments to functions
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