A Comprehensive Study of Real-World Numerical Bug Characteristics

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Abstract—Numerical software is used in a wide variety of applications including safety-critical systems, which have stringent correctness requirements, and whose failures have catastrophic consequences that endanger human life. Numerical bugs are known to be particularly difficult to diagnose and fix, largely due to the use of approximate representations of numbers such as floating point. Understanding the characteristics of numerical bugs is the first step to combat them more effectively. In this paper, we present the first comprehensive study of real-world numerical bugs. Specifically, we identify and carefully examine 269 numerical bugs from five widely-used numerical software libraries: NumPy, SciPy, LAPACK, GNU Scientific Library, and Elemental. We propose a categorization of numerical bugs, and discuss their frequency, symptoms and fixes. Our study opens new directions in the areas of program analysis, testing, and automated program repair of numerical software, and provides a collection of real-world numerical bugs.

I. INTRODUCTION

Numerical software provides the foundation for a wide variety of software applications, including safety-critical systems such as control systems for vehicles, medical equipment, and industrial plants. Libraries for machine learning (e.g., TensorFlow, scikit-learn), computer graphics (e.g., OpenGL), computer vision (e.g., OpenCV), and data analysis (e.g., Pandas) rely on numerical libraries such as NumPy [7], SciPy [24], and LAPACK [6] to perform numerical calculations. Domain-specific languages such as GNU Octave for scientific programming and R for statistical computing integrate numerical libraries to provide support for numerical computations.

Numerical software relies heavily on floating point arithmetic, which brings additional challenges in terms of software reliability and performance. Floating point is a widely used representation that approximates real numbers. By nature, floating point introduces imprecision in numerical calculations. Sources of numerical errors include extreme sensitivity to roundoff, floating-point exceptions such as overflow/underflow, and nonreproducibility across machines or even across runs on the same machine. This has led, in part, to numerical bugs that have caused catastrophic failures [2, 7, 8, 11].

Numerical bugs are those related to either the finite approximate representation of real numbers, or to mathematical aspects of the computation. Techniques have been proposed to estimate roundoff error [18, 20, 36], generate inputs that maximize errors [14], or trigger floating-point exceptions [11], and to detect accuracy [9, 12, 45] and instability problems [10, 26]. However, there is a gap of knowledge in understanding the characteristics of numerical bugs in real-world numerical software. What are the most common numerical bugs? How prevalent are these bugs? Are existing tools capable of detecting them? How are such bugs fixed? Are existing program repair tools suitable to fix them? This paper takes a first step towards answering these questions by conducting the first comprehensive study of real-world numerical bug characteristics. The goal of this paper is to study the causes, symptoms, and fixes of numerical bugs in numerical libraries, and provide a high-level categorization that can serve as a guide for researchers to develop tools for finding and fixing numerical bugs.

Empirical studies of bug characteristics have been conducted in the past to learn about concurrency bugs [27, 33], performance bugs [23, 40], and error handling bugs [13, 16], among many others. These studies have revealed patterns for both bug detection and bug fixing. To the best of our knowledge, no study thus far has focused on numerical bugs, or has considered inspecting numerical libraries, despite the reputation of being particularly subtle and error prone.

We faced a number of challenges while conducting this study. First, numerical bugs are not as numerous in general-purpose applications, which motivated us to focus our search on numerical libraries, in particular, NumPy, SciPy, LAPACK, the GNU Scientific Library (GSL) [5], and Elemental [37]. Second, examining bugs from these libraries was particularly challenging due to three main reasons: (1) the libraries use distinct version control systems and bug tracking systems (if any), (2) the libraries range from 7 to 25 years old, thus not all bugs are documented in the same manner, (3) the libraries are implemented in several different programming languages (Python, C/C++, and Fortran,) often with several languages involved in the same library. Finally, we found that, in many cases, examining and classifying numerical bugs required significant domain knowledge, and understanding of the code under inspection.

We identify and carefully examine a total of 269 numerical bugs. We propose to categorize numerical bugs into accuracy bugs, special-value bugs, convergence bugs, and correctness bugs. We find that correctness bugs are the most frequent (37%) in our dataset, followed by special-value bugs (28%), convergence bugs (21%), and accuracy bugs (14%). We discuss their characteristics, including common symptoms and fixing
strategies, and present real-world examples. Finally, based on our findings, we discuss new research directions to develop tools to improve the reliability and efficiency of numerical software.

This paper makes the following contributions:

- We identify and examine 269 real-world numerical bugs found across five widely-used numerical libraries: NumPy, SciPy, LAPACK, GNU Scientific Library (GSL), and Elemental (Sections III and IV).
- We present a categorization of numerical bugs, and discuss their symptoms and fixes (Section IV).
- We discuss new directions to test and analyze numerical programs (Section V).

The rest of the paper is organized as follows. Section II presents background on floating point, Section VI discusses related work, and Section VII concludes.

II. FLOATING POINT PRELIMINARIES

Floating point is the most common representation of real numbers. Unfortunately, floating point requires navigating many subtle tradeoffs and inevitably introduces semantics that differ from those of the reals. Indeed, many of the difficulties faced by numerical programmers are inherent in the semantics of floating point. Here we review the IEEE 754 standard [1] for floating point and its semantics.

A floating-point value is one of the following:

- A number represented as \( s \cdot c \cdot q^b \) where \( s \) is the sign (±1), \( c \) is the coefficient or significand, and \( q \) is the exponent. The base or radix \( b \) is usually 2 (binary), though the standard also describes a base 10 (decimal) representation. The significand is represented in the same base. Binary formats range in size from half precision (16 bits) to octuple precision (256 bits) in power-of-two bit widths. Most computations are carried out in single (32 bit) or double (64 bit) precision in practice.
- The infinities ±\( \infty \) representing infinite quantities. The sign of an infinity will correspond to the signs of the operands used to produce it, i.e., \( 1/0 \) and \(-1/-0 \) yield \( \infty \) while \(-1/0 \) and \(1/-0 \) yield \(-\infty \).
- The NaN value representing a result that is not a representable number, such as the result of an attempt to take the square root of a negative number. NaNs generally propagate through computations once they occur, and come in quiet and signaling varieties to implement sensible exception-generating behavior given this propagation.

Because the significand is scaled by a function of the exponent, the absolute precision of representable numbers varies with the exponent over their range. The width of the interval enclosed by a number with its last significand bit set to zero and the same number with its last significand bit set to one is called a Unit in the Last Place or ULP.

Overflow, underflow, and subnormal numbers. Results of computations that exceed the greatest representable number in magnitude in the current precision are said to overflow, and those that fall between zero and the smallest representable nonzero number are said to underflow.

\begin{table}[h]
\centering
\caption{FLOATING-POINT EXCEPTION BEHAVIOR}
\begin{tabular}{|c|c|c|}
\hline
Exception & Condition & Default Result \\
\hline
Underflow & Result between smallest normal number and zero & subnormal number \\
\hline
Overflow & Result larger than largest representable number in magnitude & ±\( \infty \) \\
\hline
Inexact & Result was not exactly representable & Rounded result \\
\hline
Invalid & Result was indeterminate or not representable as a number & NaN \\
\hline
Divide by zero & Finite, nonzero number is divided by zero & ±\( \infty \) \\
\hline
\end{tabular}
\end{table}

A subnormal number uses an exponent of zero to indicate that the exponent is the lowest representable and that the significand contains leading zero bits. This convention allows all remaining precision in the significand to be gradually exhausted as representable numbers approach zero.

Roundoff and truncation errors. Converting from a higher to a lower precision requires truncating the representations of the significand and exponent to the lengths allowed by the lower precision, which reduces both the available dynamic range and precision. The loss of precision is called truncation error while the loss of dynamic range can result in overflow.

Roundoff error is the consequence of needing to express the result of an operation in terms of representable numbers, which due to varying absolute precision across the representable range and other effects incurs errors even for operations on numbers that are themselves representable. Roundoff error of basic arithmetic operations is specified to be at most one-half of an ULP, though some implementations that favor speed (such as GPUs) violate this requirement.

Floating-point exceptions. Table I shows a summary of the floating-point exceptions. An underflow exception occurs when a result is too small to be represented by a normal number, while an overflow exception occurs when the result of an operation is too large to be represented. An inexact exception occurs when the result of a floating point operation was rounded. An invalid exception occurs when an indeterminate form, such as 0/0 is evaluated. A divide by zero exception occurs when division by zero is attempted. The environment may choose to mask exceptions, in which case the appropriate subnormal numbers, infinities or NaNs are used to represent the results and no exception is raised.

Catastrophic cancellation. Subtracting two nearly equal numbers means that most of the bits in their representations will cancel, incurring a large risk that the result will denormalize (underflow). The resulting approximation error will then propagate through the rest of the computation.

Two notable techniques intended to address the difficulties in dealing with the many undesired behaviors that can arise in computing with IEEE floating point and to track the error that accumulates in the course of computation are interval
arithmetic, standardized as IEEE 1788 in 2015 [22] and unum arithmetic [21]. Interval arithmetic represents a compact set of real numbers by its bounds, which allows tracking the set of possible solutions computed by a program, whose size measures the error. Unum arithmetic is related, and uses representations that partition the real line into exactly representable points and open sets between them. In addition to building error tracking into the representations, unum arithmetic improves the semantics of operations involving infinities or NaN versus IEEE 754 floating point.

III. METHODOLOGY

This section describes the criteria for selecting numerical libraries and the bugs to be examined, and the threats to the validity of our study.

A. Selection of Numerical Libraries

We selected five representative numerical libraries for our study: NumPy, SciPy, LAPACK, GSL, and Elemental. These libraries are characterized by their maturity (7 to 25 years old), popularity (used by thousands of projects), and active development. NumPy and SciPy are Python libraries that combine Python numerical code with wrappers for low-level routines written in C and Fortran, targeting general numerical and scientific computing, respectively. LAPACK is a C/Fortran library of low-level numerical routines, and a building block for many higher-level libraries such as NumPy. GSL mainly implements special functions and probability distributions essential to scientific computing.

Finally, we searched for public GitHub C++ repositories using keywords associated with numerical computation. We ranked the results by number of stars (project popularity). The Elemental library was ranked first. Elemental is a library that provides efficient and general linear algebra routines suitable for numerical analysis, scientific computing, and work in theoretical mathematics, via support for features such as arbitrary precision, and large-scale distributed computation.

For each library, Table I shows its language of implementation, the earliest date for which data is available, whether it is hosted in GitHub, bug tracking system used, current size (LOC), number of commits, contributors, and releases.

B. Selection and Characterization of Numerical Bugs

We chose to examine bug reports (as opposed to commits) to have access to more bug information that includes original reports from users and developer discussions. We imposed a few requirements on our bug report selection to include bugs (1) confirmed by developers (e.g., status is closed), (2) considered important (e.g., bug fix is available), and (3) more likely to be numerical bugs.

NumPy, SciPy, and Elemental are hosted on GitHub, and use GitHub’s integrated issue tracking system. This is often used by developers to track bugs, enhancements, and other tasks. Additionally, it includes GitHub pull requests. Pull requests are used by developers to contribute code (after review and approval) to a repository. LAPACK, by contrast, hosted its own development before version 3.6.1, when it was migrated to GitHub (adopting GitHub’s issue tracking system). Thus, there are two sources of bug reports for LAPACK, (1) the netlib page, which lists the bugs filed between LAPACK 3.0 (released in 2000) and LAPACK 3.6.1 (released in 2016); and (2) the GitHub repository’s issue tracker since LAPACK 3.6.1. We refer to these as LAPACK1 (before GitHub) and LAPACK2 (after GitHub) through the rest of the paper. Finally, GSL maintains a Savannah bug tracking system.

We found that all libraries, except for LAPACK1 and GSL, make use of labels to classify issues. In our selection, we filtered out any issues with labels related to build issues, documentation issues, and feature requests.

After filtering out open issues, issues without patches, and issues without relevant labels, the number of potentially interesting issues for NumPy and SciPy was still too large for manual inspection. Thus, we applied two additional filters to these projects to further refine our selection. First, we searched issue titles and descriptions for the following keywords: nan, exception, overflow, underflow, infinity, infinite, precision, unstable, instability, ringing, unbounded, roundoff, truncation, rounding, diverge, cancellation, cancel, accuracy, accurate. Second, we randomly sampled from the resulting set of issues.

We manually examined the selected bugs by reading their descriptions, comments, and any associated commits or pull requests to verify that they were numerical bugs of interest to our study. Then, we made a second pass through all bugs that passed this final selection criterion, and classified them according to the symptoms they displayed and the strategies used to implement their fixes.

C. Threats to Validity

Internal Validity. Our findings depend entirely on the set of bugs we examine. Thus, we ensured that the relevance of the initial bug selection was as high as possible by applying several filters. First, we made sure the issues and pull requests we selected were real bugs by choosing only accepted/closed issues (except for GSL where, due to limited data, we also examined issues that were open, but manually assured they had been confirmed before including them). Second, when available, we used labels from the project bug tracker as part of the selection criteria to ensure that we examined bugs considered important by project developers. Third, because we are also interested in bug fixing, we selected bugs referenced by other bugs or commits when possible, skewing our selection towards bugs with associated patches. Fourth, if the number of selected issues was too large for manual inspection, we used keywords indicative of numerical problems to select those bugs most likely to be relevant. Finally, each bug was inspected independently by each author of this paper.

External Validity. The results presented in this paper are based on only five numerical libraries, requiring special attention to select a representative sample to make generalization to other bugs in other software justifiable. To address this challenge, we selected representative, mature, and widely-used numerical libraries. Our selection includes libraries implemented in...
TABLE II
NUMERICAL LIBRARY INFORMATION

<table>
<thead>
<tr>
<th>Library</th>
<th>Language</th>
<th>Start Date</th>
<th>GitHub</th>
<th>Bug Tracker</th>
<th>LOC</th>
<th># Commits</th>
<th># Contributors</th>
<th># Releases</th>
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</thead>
<tbody>
<tr>
<td>NumPy</td>
<td>Python</td>
<td>Dec 16, 2001</td>
<td>Y</td>
<td>GitHub</td>
<td>15,366</td>
<td>15,731</td>
<td>512</td>
<td>125</td>
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<tr>
<td>SciPy</td>
<td>Python</td>
<td>Jan 28, 2001</td>
<td>Y</td>
<td>GitHub</td>
<td>823,446</td>
<td>17,012</td>
<td>479</td>
<td>91</td>
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<td>Elemental</td>
<td>C++</td>
<td>Mar 14, 2010</td>
<td>Y</td>
<td>GitHub</td>
<td>778,156</td>
<td>3,721</td>
<td>23</td>
<td>13</td>
</tr>
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<td>Website</td>
<td>1,613,856</td>
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<tr>
<td>LAPACK2</td>
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<td>Oct 26, 2008</td>
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<td>GitHub</td>
<td>1,776,339</td>
<td>1,249</td>
<td>19</td>
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<td>GSL</td>
<td>C/C++</td>
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<td>5,596</td>
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TABLE III
NUMERICAL LIBRARY ISSUES AND PULL REQUESTS

<table>
<thead>
<tr>
<th>Library</th>
<th>Issues</th>
<th>Pull Requests</th>
<th>Total Insp</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>All</td>
<td>Closed</td>
<td>w/Patch</td>
</tr>
<tr>
<td>NumPy</td>
<td>5096</td>
<td>3745</td>
<td>1335</td>
</tr>
<tr>
<td>SciPy</td>
<td>4093</td>
<td>3198</td>
<td>885</td>
</tr>
<tr>
<td>Elemental</td>
<td>123</td>
<td>85</td>
<td>18</td>
</tr>
<tr>
<td>LAPACK1</td>
<td>148</td>
<td>141</td>
<td>135</td>
</tr>
<tr>
<td>LAPACK2</td>
<td>59</td>
<td>45</td>
<td>-</td>
</tr>
<tr>
<td>GSL</td>
<td>218</td>
<td>116</td>
<td>47</td>
</tr>
<tr>
<td>Total</td>
<td>9737</td>
<td>7330</td>
<td>2420</td>
</tr>
</tbody>
</table>

TABLE IV
CATEGORYIZATION OF NUMERICAL BUGS

<table>
<thead>
<tr>
<th>Library</th>
<th>Accuracy</th>
<th>S-Values</th>
<th>Converg.</th>
<th>Correctness</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>NumPy</td>
<td>5</td>
<td>16</td>
<td>0</td>
<td>3</td>
<td>24</td>
</tr>
<tr>
<td>SciPy</td>
<td>8</td>
<td>27</td>
<td>6</td>
<td>30</td>
<td>71</td>
</tr>
<tr>
<td>Elemental</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>LAPACK</td>
<td>11</td>
<td>11</td>
<td>11</td>
<td>9</td>
<td>42</td>
</tr>
<tr>
<td>GSL</td>
<td>14</td>
<td>22</td>
<td>39</td>
<td>48</td>
<td>123</td>
</tr>
<tr>
<td>Total</td>
<td>38</td>
<td>76</td>
<td>56</td>
<td>99</td>
<td>269</td>
</tr>
</tbody>
</table>

IV. NUMERICAL BUG STUDY

The main purpose of this numerical bug study is to answer the following research questions:

R1. How frequent are numerical bugs?
R2. How can we group numerical bugs into categories that share common causes and patterns, and how frequently do bugs in each category occur?
R3. What other characteristics of numerical bugs can we identify to inform building tools?

We examined a total of 828 bugs (issues and pull requests) from five numerical libraries (NumPy, SciPy, Elemental, LAPACK, and GSL). Table III lists the total number of issues, and pull requests (PRs) per library. The column “Closed” refers to the number of issues/PRs with status closed. The column “w/Patch” indicates the number of closed issues/PRs that include patches, and the column “Label” indicates the number of closed issues/PRs with patches that were selected based on their labels.

For SciPy and NumPy we provide two numbers. The second number is the number of labeled issues/PRs in which relevant numerical keywords (see Section III) were found. From these, we randomly selected 80 issues and 20 PRs from each of NumPy and SciPy. We inspected all 218 bug reports for GSL, and all closed 85 issues and 100 PRs for Elemental. In total, we inspected 629 issues and 199 PRs. We use issues/PRs and bugs interchangeably in the rest of this paper.

We found 269 numerical bugs in the 828 bugs inspected, and developed a categorization of numerical bugs that consisted of four groups: accuracy, special value, convergence, and correctness. Table IV shows the distribution of each kind of bug across the five libraries studied. Next we describe the characteristics of each bug category.

Finding 1: 32% of the bugs examined are numerical bugs. Based on our observations, we propose four categories for numerical bugs: accuracy, special value, convergence, and correctness.

A. Accuracy Bugs

We classified bugs as accuracy bugs when precision loss due to rounding or truncation errors led to an incorrect result. Out of the 269 numerical bugs, we found 38 accuracy bugs across four numerical libraries. These bugs were found mostly in decomposition and eigenvalue computation routines in LAPACK, and in the core components of GSL, SciPy, and NumPy. We found that accuracy bugs often fell into one of three subcategories:

1. Insufficient Precision Data Type. To determine the precision of a variable one must take into account the range of values to be stored. While using too much precision can cause performance degradation and/or increase in memory usage, using too little precision can cause precision loss that may lead several of the most commonly used programming languages for numerical code and addressing a comprehensive range of subtypes of numerical code at levels of abstraction from low-level arithmetic and linear algebra to higher-level, large-scale scientific computing and number theory.
A large condition number indicates that the problem itself is ill-posed: the condition number is much larger than the order of an expression as shown in Fig. 2, the developers found in a result, the issue may be inherent to the problem, as it is much smaller than 1. High precision data types would be necessary to achieve correct behavior.

(2) Inaccurate Arithmetic Expressions. Floating-point arithmetic expressions must be carefully crafted to minimize the generation and propagation of roundoff errors. Fig. 2 shows an example where the order in which arithmetic operations are computed leads to precision loss. The bug is fixed by introducing two temporary variables and breaking the original arithmetic expression into three separate expressions to enforce the required order of computation. Fig. 3 shows another example: two expressions that suffer from catastrophic cancellation are replaced with different but equivalent expressions.

(3) Ill-Conditioned Problem. When a large numerical error is found in a result, the issue may be inherent to the problem, as it would appear regardless of the algorithm used. The condition number of the problem is the key to make this distinction. A large condition number indicates that the problem itself is sensitive to numerical errors. Fig. 4 shows an example of an ill-conditioned problem. After examining the contribution order of an expression as shown in Fig. 2 the developers discussed the problem further and recognized that the problem is ill-conditioned – its condition number is much larger than 1 when \( v \) is much smaller than 1. High precision data types would be necessary to achieve correct behavior.

Detection and Fixing Automation. In the bugs we examined, backward error analysis was often used in the detection of accuracy bugs. For example, to test a division on floating-point numbers, \( q, r = \text{divmod}(a, b) \), the accuracy of the quotient \( q \) and remainder \( r \) can be determined by comparing \( q = b + r \) and \( a \). A similar technique can be used to test decomposition and eigenvalue computation routines. In these cases, the two resulting matrices should be orthogonal in theory. A problem is revealed if their product greatly deviates from the unit matrix. Such techniques could be used for bug detection. Input generation is another important aspect in detecting accuracy bugs, however we did not find any mention of input generation when examining the bug reports. Finally, we found that the first two subcategories suggest strategies for fixing accuracy bugs: switching to higher precision, and transforming arithmetic expressions to improve their precision.

Finding 2: Accuracy bugs are the least frequent numerical bugs in our dataset (14%). Techniques such as backward error analysis could be used to automatically detect these bugs. Furthermore, we identify two common strategies to fix accuracy bugs: using higher precision, and reordering arithmetic expressions. Input generation to detect accuracy bugs remains a challenge.

B. Bugs Related to Special Values

In this paper, we refer to signed zero, subnormal numbers, infinities, and NaNs (Not a Number) as special values. Unlike normalized floating-point numbers, special values are given a special encoding in the floating-point representation system. Moreover, arithmetic operations on special values follow irregular rules with subtle implications. We denote a bug as
A user reported NaN value bug is overflow/underflow, which can lead to NaN values, producing incorrect results, causing infinite loops, etc.

GESVD NaN bugs are caused by a variety of problems, and often require NaN if the input array contains a NaN. Furthermore, the function is modified to immediately return a NaN − 1 \ldots 1 \ldots 1 \ldots 1 NaN[49x88] checks whether NaN[49x424] − 1 is larger. Then, it checks whether NaN is larger than −2, which also fails, and −2 is returned. To fix this bug, a NaN check is added to check the array for NaNs. Furthermore, the function is modified to immediately return a NaN if the input array contains a NaN value.

(2) Overflow/Underflow. Another important type of special-value bug is overflow/underflow, which can lead to NaNs. These bugs are caused by a variety of problems, and often require domain specific knowledge for their detection. Fig. 6 describes an underflow bug in the LAPACK library that results in NaNs. A user reported NaN values in the result when calling routine GESVD to compute the singular value decomposition of a matrix with all elements set to 1. The input matrix leads to denormalized numbers when bidiagonalized in GESVD. This matrix is eventually passed to routine LASQ3. In LASQ3, T is computed by taking half of (Z(nn − 7) − Z(nn − 3)) + Z(nn − 5), where nn is a local scalar, underflowing and becoming 0. NaN values are then produced in S when dividing T. A fix for this bug is proposed by strengthening the conditions for further computation on T, i.e., avoiding the computation of S when T underflows. This fix required domain specific knowledge.

Detection and Fixing Automation. NaNs are designed to denote the results of “invalid” floating-point operations, e.g., 0/0, without interrupting execution. Furthermore, NaNs are often used to represent missing data, which can lead to ambiguity. Both uses cause errors due to the idiosyncratic behaviors of computations on NaNs and other special values, and their non-local propagation. An approach to detect special-value bugs is to feed NaN inputs to functions to observe where and how they subsequently fail. This could be used to reveal problems with NaN checks or their absence. On the other hand, generating inputs to reveal underflow/overflow errors is, however, difficult to automate, as it requires domain-specific knowledge. Finally, the main challenge in automating bug fixing is to determine when to check for special values, and what to do in their presence.

Finding 3: We find that 28% of the numerical bugs are special-value bugs. These bugs mainly involve NaN checks and overflow/underflow conditions. An initial approach to detect missing NaN checks is to use NaN inputs. Generating inputs to expose overflow/underflow remains a challenge.

C. Convergence Bugs

We define convergence bugs as bugs where an iterative or series approximation diverges or converges too slowly due to numerical problems such as magnified roundoff or truncation errors. This is related to numerical instability, i.e., the output is sensitive to small variations in inputs or intermediate quantities. Consequently, small errors introduced by floating-point approximations drive the output far from the correct value. This can be complicated by interactions with instability around conditional tests, where vanishingly small differences in a quantity involved in a test can cause different control paths to be followed. An example is the termination of a loop that intends to continue an iterative approximation until an error estimate goes below a given error tolerance.

We find that 56 out of 269 numerical bugs correspond to convergence bugs; 39 were found in GSL, 11 in LAPACK, and 6 in SciPy. We did not find any convergence bugs in the sampled issues from NumPy or Elemental. This was unremarkable in the case of NumPy because NumPy focuses mainly on low-level linear algebra data structures, and operations on these are delegated to wrapped algorithms from other packages. Elemental includes support for arbitrary-precision arithmetic. Arbitrary-precision arithmetic avoids convergence issues by scaling precision according to the demands at each point in a computation.
Convergence bugs fall into one of the following scenarios:

- The approximation algorithm uses a problematic approximation formula that yields a wrong result.
- Numerical issues in an iterative approximation cause an infinite loop that leads to a program crash.
- Special values such as NaNs are involved in divergent behavior. We classify this as a convergence problem yielding a wrong result rather than a special-value issue because it is more specific to do so.

An example of a convergence bug is illustrated in Fig. 7. A user noticed an error larger in magnitude than the result itself in the output of the hypergeometric special function in the regime of large negative $a$, positive $b$, and large positive $x$ parameters. Another user noted that the Kummer transformation used for $x < 100$ returned correct results for larger $x$ as well, and proposed a fix to use it by default in this regime for all values of $x$, which was accepted.

In general, the symptom revealing a convergence bug was usually the output of wrong results. Occasionally, failure to converge would result in a non-terminating loop, hanging the program, which we classified as a crash.

Detection and Fixing Automation. Because failures to converge are due to issues in the quality of a numerical approximation, these require domain-specific knowledge to address, and fixes usually involve using a better approximation technique. In principle, running programs with arbitrary-precision arithmetic could help to automate finding such issues. Since these bugs are among the most common in scientific computing packages that implement special functions, and probability distributions, such a tool could be highly valuable. Unum arithmetic could be especially interesting in this context because it combines aspects of interval-based error tracking with adaptive precision.

Finding 4: We found that $21\%$ of the numerical bugs are convergence bugs. Diagnosing convergence bugs requires domain-specific knowledge. Adaptive use of interval and arbitrary-precision should be investigated further. In this context, Unum arithmetic is especially interesting since it combines a form of interval-based error tracking with adaptive precision.

D. Correctness Bugs

A correctness bug is caused by any error in the implementation of an algorithm that have to do primarily with its mathematical or algorithmic structure. Correctness bugs are the most type of numerical bug; $99$ out of $269$ numerical bugs are correctness bugs. Correctness bugs have the greatest variety of all types, and ranged from typographical errors in transcribing a formula from a reference, to using an approximation formula that yields a wrong result rather than the correct result. We classified correctness bugs into the following subcategories:

- Errors in the initialization or updates in iterative solvers that resulted in problems other than a failure to converge to the correct result.
- Errors in conditional tests that resulted in the wrong function approximation being used for the given point in the domain.
- Errors involving vector and matrix data data types, such as element type errors and incorrect array dimension.
- Violations of assumed numeric semantics due to compiler optimizations.

Fig. 8 shows an example of a numerical correctness bug related to error initialization found in SciPy. The bug is found in code wrapping a call to a Fortran routine for Sequential Least-Squares Programming, where there is an erroneous attempt to use dummy values of $\pm 1e12$ for constraint bounds passed to the solver. This resulted in scaling problems in the solver due to the large range of the constraints and also precluded finding solutions outside those bounds even when they existed in the given problem. The underlying Fortran routine in fact supported using NaN in the place of bounds for unbounded parameters.

```c
int gsl_sf_hyperg_1f1_e(const double a, const double b,
                        const double x,
                        gsl_sf_result * result) {
    ...
    - else if(a < 0.0 && fabs(x) < 100.0) {
        /* Use Kummer to reduce it */
        /* to the generic positive case... */
        gsl_sf_result Kumer_1F1;
        int stat_K = hyperg_1F1_ab_pos(b-a, b, -x,
                                       Kumer_1F1);
        int stat_e = gsl_sf_exp_mult_err_e(x,
                                           GSL_DBL_EPSILON * fabs(x),
                                           Kummer_1F1.val,
                                           Kummer_1F1.err,
                                           result);
        return GSL_ERROR_SELECT_2(stat_e, stat_K);
    }
    ...
}
```

Fig. 7. GSL issue #28718: an example of a convergence bug.
problems, and once that fix was made (and an array bounds error introduced by the initial fix was then addressed) the routine worked as expected.

**Detection and Fixing Automation.** Correctness bugs were most often discovered through the symptom of an incorrect result being returned. The majority of these were discovered by users noticing incorrect results in the course of their work and comparing the library results to other implementations of the same feature, usually in less efficient but more rigorous packages that include such features as arbitrary-precision arithmetic, for example PARI/GP\[3\]. This suggests that differential testing against such a package could be an effective bug-finding approach. A minority were discovered through test cases failing. These were often platform or build specific, and were the fault of the compiler violating semantic assumptions implicit in the code under certain conditions. This suggests the approach of using a database of platform, build, and environment dependent code under certain conditions. This approach, for example PARI/GP[3], suggests that differential testing against such a package could be an effective bug-finding approach. A minority were discovered through test cases failing. These were often platform or build specific, and were the fault of the compiler violating semantic assumptions implicit in the code under certain conditions. This suggests the approach of using a database of platform, build, and environment dependent behavior to scan code for instances of patterns that differ in their behavior across targets.

In general, correctness bugs required the most domain-specific knowledge of all types to fix, given that they were most related to the mathematical structure of the problem at hand and the idiosyncrasies of the language and environment.

**Finding 5:** Correctness bugs are the most common numerical bugs, with 37% of numerical bugs falling into this category. Correctness bugs are extremely challenging to detect. Differential testing may be a good method to detect these bugs.

**E. General Bug Symptoms and Opportunities for Automation**

We identified three common symptoms of numerical bugs: **wrong results**, **crashes**, and **bad performance**. Table VI shows their distribution across libraries. We found that the majority of numerical bugs (77%) are revealed by producing wrong results. This is followed by crashing the program (13%), and causing bad performance (10%). For all libraries except Elemental, producing wrong results was the most common symptom of a numerical bug. The second most common symptom was program crashes for NumPy and SciPy, and bad performance for Elemental, LAPACK, and GSL.

We also classified bugs according to whether detection or fixing could be automated. Table VI shows our classification, and the distribution across libraries. “Pattern” describes bugs that could be detected or fixed by applying a simple pattern, “Analysis” refers to bugs that could be potentially detected or fixed automatically after non-trivial analysis of the code, and “Domain Specific” are bugs that require domain specific knowledge to be detected or fixed. We found that very few bugs (4%) can be detected using simple patterns (e.g., matching small AST fragments to repair problematic order of operations). However, we found that a considerable number of bugs (29%) might be detected automatically with program analysis techniques (e.g., dataflow analysis to aid in estimating output error from intermediate roundoff errors). In the case of automated bug fixing, fewer bugs could be fixed by applying patterns (2%), or analyzing code (17%); a large majority of fixes were domain specific. Note that we considered only 183 bug fixes in our study.

**Finding 6:** The most common symptom for numerical bugs is wrong results, which is observed in 77% of the bugs. This is followed by crashes with 13%, and bad performance with 10%. About 80% of the numerical bugs required domain specific knowledge to be fixed.

**V. LESSONS LEARNED**

(1) **Frequency of Numerical Bugs.** Even in the projects we examined, which focus exclusively on numerical code, 32% of the reported issues were numerical bugs. We speculate that this may be due to the relative maturity of these projects, and that the essential functionality is already in place and thoroughly debugged. Because of the widespread use and maturity of these libraries, and their tendency to be implemented by highly-skilled experts, we would also expect that the bugs most relevant to this study were discovered and fixed early in the project lifecycle, if they appeared at all, thus we may need to look for historical bug data that far predates the migration of these projects to GitHub, if they appear on GitHub at all. Finally, numerical bugs can also be present in clients of numerical libraries, and other applications (e.g., [28]). It would be interesting to investigate whether our findings apply to code other than numerical libraries.

(2) **Current Tool Usage.** We did not find any indication during our manual inspection that bug detection tools were used by developers or users. In most cases, users seemed to find inputs that exposed unexpected behavior almost by chance. There was also no indication that developers of these libraries...
we found a few users who determined that a library was
we could apply those patterns to detect unknown bugs in the
identified in this study.
(e.g., tools that find divergences [15]) are able to find the bugs
we identified in this study. Tools such as Herbie [36] and Precimitious [38] could be applicable in these scenarios.

(4) Testing and Input Generation. In our manual inspection,
we found a few users who determined that a library was
producing an incorrect result because they had performed
the same numerical operation in a more rigorous but less
efficient library, and found a mismatch in the results. This
suggests that differential testing of numerical libraries could
be particularly beneficial for numerical software for which
oracles are often difficult to obtain. This would be particularly
useful to detect many of the bugs that we classified as requiring
domain-specific knowledge (the majority in this paper). Even
in the absence of a known-good implementation, differential
testing of numerical libraries would help to detect many of
the most difficult bugs by simply finding mismatching results
across different numerical libraries, taking advantage of the
tendency of different implementations to fail in different ways
in challenging tasks. We also found that techniques for input
generation (e.g., [14, 45]) are in great need to uncover many of
the problems described throughout this paper.

(5) Program Analysis. Program analysis tools could be de-
veloped to automatically detect a good number of numerical bugs,
including special-value bugs, accuracy bugs, and convergence
bugs. In particular, current challenges in the estimation of
roundoff errors (e.g., treatment of loops in [17, 42]) present
interesting problems that will have a great impact on being
able to find a variety of numerical bugs. In the case of dynamic
tools, the main challenge will be to produce results that can be
generalized to many program runs while imposing low runtime
overhead. A delicate balance between static and dynamic
approaches is needed.

(6) Automated Bug Fixing. As with other kinds of bugs,
automated bug fixing of numerical bugs seems to be the most
challenging. The first step would be to apply the state-of-the-art
(e.g., [31, 32, 34]) in automated bug repair to see if any of the
bugs we identified could be fixed. For certain narrowly-defined
cases, simple pattern matching may provide some low-hanging
fruit in the meantime.

VI. RELATED WORK

Empirical Studies. Previous empirical studies have examined
a variety of software systems, and characterized their defects
and associated information on various dimensions [19, 23, 33,
34, 43]. We summarize some of the most related studies that
have inspired our work. A study of performance bugs [23]
examined 109 performance bugs from Apache, Chromium,
GCC, Mozilla, and MySQL, classifying them according to
their root cause, how the bug was introduced, how it was
exposed, how it was fixed, and its location in the code. A
more recent study [40] examined 98 fixed performance bugs
in 16 popular client-side and server-side JavaScript projects,
finding eight common root causes. In our study, we found
that about 10% of numerical bugs have performance-related
symptoms. To the best of our knowledge, previous studies on
performance bugs did not find instances of numerical bugs
causing performance problems.

Similar studies have focused on other aspects of software.
For example, Dietz et al. [19] investigate integer overflow bugs
in C/C++ programs by performing dynamic checking on the
SPEC CINT 2000 benchmarks and also identifying undefined
integer overflows in widely used open source software. Our
study instead investigates floating-point numerical bugs, and in
addition to overflow (and underflow) develops a comprehensive
categorization of bugs empirically. In recent studies (e.g.,
[29, 30, 35]), the authors have developed tools to address
specific bug types using pattern-matching based detection and
correction techniques informed by empirical analyses, which
in part motivated our empirical study.

Tools for Numerical Code. A variety of tools have been
developed to improve the reliability and performance of
numerical applications. For example, techniques have been
devised to estimate roundoff errors. FPTaylor [42] focuses
on providing a tight overapproximate estimate on roundoff
errors by rigorously handling the transcendental functions
using Symbolic Taylor Expansions. Darulova and Kuncak [17]
present a programming model that provides real data type for
programmers and guarantees a sound compilation to finite-
precision implementation that meets the desired precision.
At the same time, a series of dynamic tools have been developed to test and optimize numerical code. For example, techniques [14, 45] have been proposed to generate inputs that lead to large roundoff errors that can be used to test numerical code. Tools for precision tuning [25, 39] dynamically search over the types of variables or instructions to find a mixed precision configuration that (1) produces an accurate result with respect to an error threshold, and (2) improves performance. Herbie [36] rewrites floating-point arithmetic expressions with mathematically equivalent alternatives in order to improve the accuracy of the computations.

Though promising, the above-mentioned tools, as many others, remain narrow in scope and have not been adopted by real-world applications. We hope that our study on real-world numerical bugs can provide context to improve existing tools and to inform the design of future tools so that they engage better with the full depth and breadth of numerical programming problems in the real world.

VII. CONCLUSIONS

This paper presented the first comprehensive study of real-world numerical bug characteristics. We examined 828 issues and pull requests from a diverse set of numerical libraries: NumPy, SciPy, Elemental, LAPACK, and GSL. From these, we identified and carefully examined 269 numerical bugs. We found that numerical bugs can be largely categorized into four groups: accuracy bugs, special-value bugs, convergence bugs, and correctness bugs. Correctness bugs, with 37%, comprise the single most common category, and are also the ones that require the most expertise. Correctness bugs are followed by special-value bugs, convergence bugs, and accuracy bugs with 28%, 21%, and 14%, respectively.

We discussed the characteristics of numerical bugs. We found that the most common symptom for numerical bugs are wrong results, followed by crashes and bad performance. We discussed the opportunities to automate detection and fixing of numerical bugs. While merely using patterns applies to few bugs, there is still promise in these being applicable to a large number of libraries and library clients. We found that many bugs could potentially be detected using program analysis, and that there may be opportunities in the area of automated bug fixing as well. As for existing tools, we did not find evidence that suggests the current use of testing/analysis tools by library developers or users. Thus, more work is also required to facilitate the adoption of numerical tools in the real world.

ACKNOWLEDGMENTS

We thank the anonymous reviewers for their insightful comments. This work was supported in part by NSF grant CCF-1464439, and a Hellman Fellowship.

REFERENCES


