

Methodological Aspects of Studying the Accuracy of Computer Calculations in Applied Problems

Oleh Vietrov¹, Olha Trofymenko², Vira Trofymenko¹ and Maxim Hryhorov¹

¹ Vasyly Stus Donetsk National University, 21, 600-richchia str., Vinnytsia, 21021, Ukraine

² University of Connecticut, 341 Mansfield Road, Storrs, CT 06269, USA

Abstract

The study is dedicated to considering some examples of computer calculations that are completely correct from the point of view of the standards of computer work with numbers and arithmetic operations, the result is incorrect to a human performer. It's demonstrated that mathematically correct calculations are often impossible to reproduce correctly within the IEEE-754 standard due to the fundamental limitations of the memory allocated to represent a specific number. The authors focused on the study of the specified problem using the example of the numpy module, as one of the main software tools for modern scientific calculations. The work has methodological value in the professional training of specialists in Computer Science.

Keywords

Computer calculations, IEEE-754 standard, numpy

1. Introduction

The problem of reliability of computer calculations is one of the fundamental problems of Computer Science [1], as it lies at the intersection of applied mathematics on the one hand, and physical and technical limitations of computer technology on the other. The avoiding the fundamentals of binary arithmetic and the principles of the standard for representing numbers in computer memory can significantly affect the correctness of both theoretical research (if computer technology was used for modeling) and simply the quality of the product when developing application programs.

The problems that can arise due to incorrect representation in computer memory are well known. Sometimes they are subtle problems that do not have a significant impact in a qualitative sense on a particular result. Therefore, in application activities, floating-point computing problems and features of IEEE-754 standard are often overlooked by software developers as well as academic researchers. However, there are notorious cases when careless handling of computer representation of numbers led to serious tragedies. A well-known example of the tragic consequences of such problems is "The Patriot Missile Failure" [2-3]. The main problem was that the time value in tenths of a second was multiplied by a factor of 0.1 to get a representation of time in seconds. This calculation was done using a 24-bit fixed-point register. The Patriot battery lasted about 100 hours and the accumulated error was about 0.34 seconds. One can also recall the precedent of "The Explosion of the Ariane 5" [4-5]. As a result of computer calculations, a 64-bit floating-point number was converted to a 16-bit signed integer. The number was greater than 32,768, and so the conversion failed. An error in the system for calculating the horizontal velocity of the rocket relative to the platform resulted in damage estimated at 500 million dollars. Some examples of real losses caused by rounding errors or problems in representing numbers in computer memory are given in [6].

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✉ o.vietrov@donnu.edu.ua (O. Vietrov); olha.trofymenko@uconn.edu (O. Trofymenko); v.trofymenko@donnu.edu.ua (V. Trofymenko); hryhorov.m@donnu.edu.ua (M. Hryhorov)

ORCID iD 0000-0002-5125-9632 (O. Vietrov); 0000-0002-3925-5815 (O. Trofymenko); 0009-0005-8094-227X (V. Trofymenko); 0000-0001-6817-2624 (M. Hryhorov)



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The limitation on the amount of memory allocated by computer technology for number processing imposes fundamental limitations on the possibilities and logic of the organization of computer calculations. It's also requires the involvement of specific mathematical research methods.

The standard and most popular tool for computer calculations, especially in machine learning tasks, is the Python programming language, in particular with its powerful extension NumPy module. It allows you to efficiently work with large multidimensional arrays and matrices, along with a large library of mathematical functions. The NumPy module provides much wider possibilities for working with mathematical functions and objects compared to the math module. The NumPy is an effective tool for providing complex mathematical calculations not only in the tasks of machine learning and data analysis, but is also an indispensable component in the implementation of a large volume of computer calculations in a wide class of modern engineering and scientific tasks [7-10].

The investigation considers the main aspects related to the problems of computer calculations within the IEEE-754 [11] standard, the main technical standard format for representing floating-point numbers (floating-point numbers) (discussing possible alternatives to the IEEE-754 standard, such as Unum [12] and Posit [13-14] go beyond the scope of the presented work).

The history of the development of computing and the basics of the theory of computing with floating-point numbers are described in [15-16]. Important related issues of floating-point computing are presented in [17-18]. Recently, the research in the direction of computer-assisted proof for various classes of mathematical problems [19] is more developed. In this work, the authors touch on possible incorrect cases of the possible use of proof calculations in case of failure to take into account certain features of the representation of numbers in the computer memory.

The presented work is a continuation of the authors' research [20-21]. Previously, the authors investigated rather complex cases of violation of the correctness of computer calculations, the example of Ramp [22] and the sequence of Müller [15]. The works of [20-21] investigated the mathematical aspects of computer calculations, in particular the convergence and stability of computer calculations. The authors focused more on the methodological principles of teaching the topic of accuracy of calculations for the Computer Science specialty students in the presented work. Based on the teaching experience, the authors believe that a detailed study of the problem of the incorrectness of computer calculations on trivial examples (rather than specially designed ones) will allow students to take a more serious and attentive approach to the problems of computer calculations.

2. Methods

Let's consider the numeric data types of the NumPy library, one of the most popular Python libraries for scientific computing. Figure 1 shows the hierarchical diagram of the `numpy.generic` data class, the base class for numpy scalar types. We not consider components of `numpy.generic` like `numpy.bool_`, `numpy.object_`, `numpy.datetime64` or `numpy.flexible`.

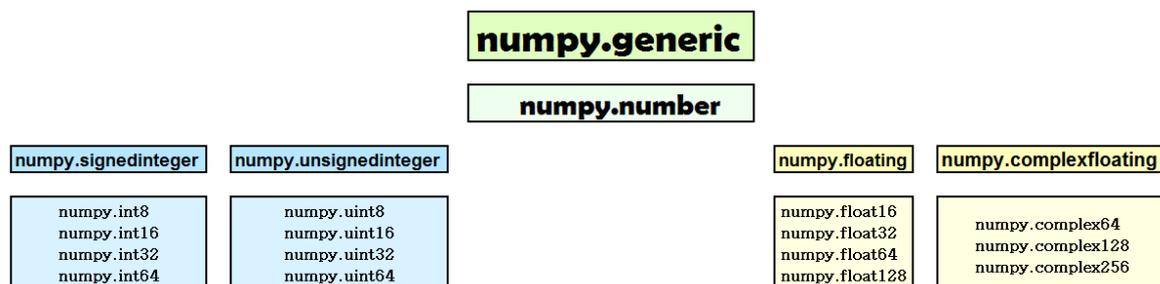


Figure 1: Numpy number types

Floating point numbers according to the IEEE 754 standard are presented in the form

$$number = (-1)^s \times 1.M \times 2^E$$


```

3     iteration_count_eps = 1
4     mach_eps = float_format(1)
5     while float_format(1) + float_format(mach_eps)\
6         /float_format(2) != float_format(1):
7         iteration_count_eps += 1
8         mach_eps /= float_format(2)
9     return mach_eps, iteration_count_eps
10
11    def machineZero(float_format = float):
12        iteration_count_zero = 0
13        mach_zero = float_format(1)
14        while float_format(mach_zero)\
15            /float_format(2) != float_format(0):
16            iteration_count_zero += 1
17            mach_zero /= float_format(2)
18        return mach_zero, iteration_count_zero

```

Result:

Machine Epsilon

```

<class 'numpy.float16'>: (0.000977, 11)
<class 'numpy.float32'>: (1.1920929e-07, 24)
<class 'numpy.float64'>: (2.220446049250313e-16, 53)
<class 'numpy.longdouble'>: (1.084202172485504434e-19, 64)

```

Machine Zero

```

<class 'numpy.float16'>: (6e-08, 24)
<class 'numpy.float32'>: (1e-45, 149)
<class 'numpy.float64'>: (5e-324, 1074)
<class 'numpy.longdouble'>: (4e-4951, 16445)

```

We see that a specific machine epsilon, like a machine zero, is not fundamental. The order of given numbers is important. The value of the `iteration_count_eps` variable is the negative power order $2^{-\text{iteration_count_eps}}$. As we can see, for the machine epsilon for the corresponding type of floating point numbers, the `iteration_count` value is one more than the number of bits allocated for the mantissa value for the corresponding type. This makes sense because it implies the precision limits for the corresponding numeric type.

As for the results for machine zero, the given values are the smallest numbers below which the computer already perceives as zero.

That is, in fact, the machine zero is a number $2^{-(\text{iteration_count_zero}+1)}$. It is obvious that it is possible to obtain the order of the machine zero without computer calculations using the formula

$$\text{mantissa} + 2^{\text{exponent}-1},$$

where the exponent and the mantissa determine the number of bits for the corresponding data type.

3. Results and Discussion

3.1. Restrictions on calculations in integers

Let's consider one interesting example of working with integers when overflowing a bit grid.

This problem itself is well known, but when training specialists, it is important to demonstrate that the results obtained are incorrect to a human programmer, but are nevertheless absolutely correct from the point of view of executing the program within the framework of existing standards. A simple example is the calculation of the value of the factorial of some natural number n . With implementing directly in Python (the factorial function from the `math` module), there are no problems with accuracy. Python implements the `BigInt` [24]

3.2. Homer Simpson's numbers

Let's consider another example of manipulating integer formats. The images in Figure 3 are stills from the episode "The Wizard of Evergreen Terrace" [26] and the episode "Treehouse of Horror VI. Homer3 (Homer Cubed)" [27] of the popular animated series The Simpsons.

Mathematical statements relating to Fermat's Great Theorem will be true when checked with a calculator [28]. Let's consider the first example when working with numeric data types from the numpy module.

Of course, the actual numerical values do not match

$$3987^{12} + 4365^{12} = 63976656349698612616236230953154487896987106$$

$$4472^{12} = 63976656348486725806862358322168575784124416$$

Note that an attempt to convert any number to int32, int64 (uint32, uint64) types generates an OverflowError error.

Direct conversion to float32 also generates an OverflowError, so let's try to consider a mathematically identical expression

$$398.7^{12} + 436.5^{12} \neq 447.2^{12}$$

Now the result of the operation in Python (`398.7**12 + 436.5**12 == 447.2**12`) will be True. Indeed, it is fashionable to write within the IEEE-754 standard

Arithmetic expression:	$398.7^{12} + 436.5^{12}$
Correct value:	63976656349698612616236230953154.487896987106
Float32 format:	63976654187609440353486161051648.00
Binary format:	0 11101000 10010011101111111101110

Arithmetic expression:	447.2^{12}
Correct value:	63976656348486725806862358322168.575784124416
Float32 format:	63976654187609440353486161051648.00
Binary format:	0 11101000 10010011101111111101110

That is, the reason lies in discarding the lower bits when converting a number to the float32 format.

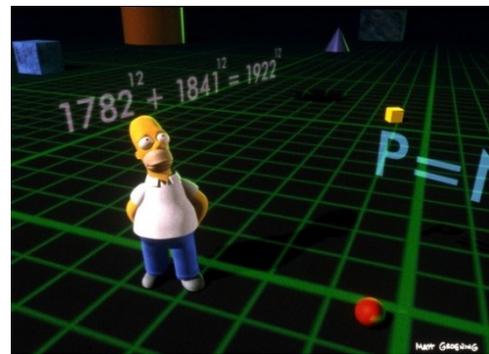
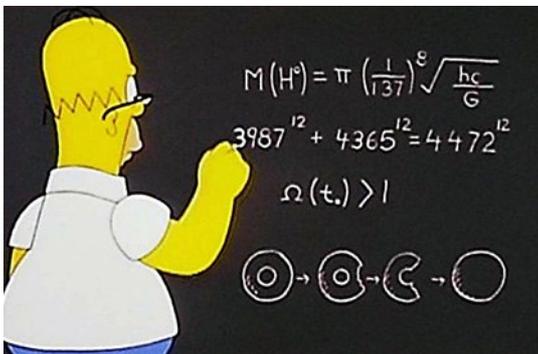


Figure 3: Homer Simpson's example

Let's consider the same problem, but staying within the framework of integer formats.

For example, for $n = 5$ for the int32 format, more than 1400 triples of natural numbers (A, B, C) can be found, so that when calculating `int32(A**5) + int32(B**5) == int32(C**5)` would return a boolean value of True.

The maximum value of the parameter C: $C = 6208$, and as can be seen from the Table 4, several pairs (A, B) can correspond to one value of C. The explanation for this is simple: different large integers (more than 4 bytes) due to the discarding of the high-order bits in the int32 format can have the same value. For triples from the Table 4 (32, B, 6208) we have

$$\text{int32}(6208^{**5}) = 1073741824,$$

$$\text{int32}(992^{**5}) = \text{int32}(5088^{**5}) = 1040187392, \text{int32}(32^{**5}) = 33554432.$$

Similarly for the triples (64, B, 6208) we have

$$\text{int32}(B^{**5}) = 0, \text{int32}(64^{**5}) = 1073741824.$$

Table 4
 $C^2 = B^2 + A^2$ (float32)

C	B						A
	992, 5088						32
	128,	256,	384,	512,	640,	768,	
	896,	1024,	1152,	1280,	1408,	1536,	
	1664,	1792,	1920,	2048,	2176,	2304,	
6208	2432,	2560,	2688,	2816,	2944,	3072,	64
	3200,	3328,	3456,	3584,	3712,	3840,	
	3968,	4096,	4224,	4352,	4480,	4608,	
	4736,	4864,	5120,	4992,	5248,	5376,	
	5504,	5632,	5760,	5888,	6016,	6144	

Most of the examples for $n = 5$ look artificial and any user will immediately understand that the obtained result is incorrect from a mathematical point of view. But you can choose an example when an untrained user can mistakenly perceive the result as correct, for example, implementing C++ programs for the standard type `int` (4 bytes). From our point of view, this is the example of $A = 1504$, $B = 2960$, $C = 4496$, $n = 5$. At the same time, it is interesting that the values of the expressions A^5 and B^5 in the `int32` format are generally negative numbers:

```
int32(1504**5) = -570425344,
int32(2960**5) = -1584398336,
int32(4496**5) = 2140143616.
```

In the additional code in `int32` format, we can write

```
(-570425344)10 = (11011110000000000000000000000000)2
(-1584398336)10 = (10100001100100000000000000000000)2
```

In the binary code, the sum of these numbers will have a length of 33 bits and is equal to

```
(-570425344)10 + (-1584398336)10 = (10111111100100000000000000000000)2
```

Discarding the most significant bit (33 bits), we get the result

```
(01111111100100000000000000000000)2 = (2140143616)10.
```

3.3. Another simple examples

Let's move on to consider some typical examples of incorrect behavior of computational algorithms about working with floating point numbers.

Consider the following problem: it is necessary to find such a minimum value of n that

$$\frac{1}{m} + \frac{1}{n} = \frac{1}{2020}, \quad \begin{matrix} m \in N \\ n \in N' \end{matrix}, \quad n > m$$

This problem is an example of Diophantine equation. In a general sense, the Diophantine equation is an equation in which only integer solutions are allowed.

The program for solving this equation is presented in listing #2.

Listing #2

```
1 import numpy as np
2 def mathExpr (num_format):
3     value = num_format(1/2020)
4     n = 1
5     while True:
6         n1 = num_format(1/n)
7         for m in range(1, n):
8             if n1 + num_format(1/m) == value:
9                 return n, m
10            n += 1
11 float_formats = (np.float16, np.float32, np.float64, np.float128)
```

```

12 for form in float_formats:
13     print(f'{form}:', mathExpr (form))

```

```

Result: <class 'numpy.float16'>:      n = 4039, m = 4035
        <class 'numpy.float32'>:      n = 4041, m = 4039
        <class 'numpy.float64'>:      n = 4545, m = 3636
        <class 'numpy.longdouble'>:   n = 6060, m = 3030

```

As a result, we got four different answers depending on the format of the floating point numbers. At the same time, the pairs (4545, 3636) and (6060, 3030) are the correct solution to the equation.

It is easy to show that $n = 4545$, if we look for the minimum value of n . That is, when using the float16 and float32 formats, we will get incorrect answers, and in the case of the float128 format, we will get a correct answer from a mathematical point of view, but we will skip over the minimum possible value of n ($n = 4545$), which satisfies the problem. We can engage the specialized apparatus of computer computation to improve the accuracy of computation. Let's try to increase the accuracy of calculations in Python using a special decimal module [30] by adding a decimal.Decimal element to the float_formats tuple. However, when trying to execute the program, we will get into an infinite loop, and the task of finding an exact match of values can be considered as failed.

We can correct this situation, for example, using the isclose method from the math module. To do this, in listing #2, line 8 must be replaced with the command *if math.isclose(n1+num_format(1/m), value, rel_tol=1e-9)*, and in this case, the float128 and decimal.Decimal format will already have $n = 4545$, $m = 3636$. Let's change line 3 in listing #1 to the command `value = num_format(1/10)`, and after starting the program, we will get the result:

```

<class 'numpy.float16'>: n = 30, m = 15
<class 'numpy.float32'>: n = 35, m = 14
<class 'numpy.float64'>: n = 30, m = 15
<class 'numpy.longdouble'>: Infinite loop
<class decimal.Decimal'>: Infinite loop

```

Obviously, the answer to the problem is the pair $n = 30$, $m = 15$ (the pair $n = 35$, $m = 14$ is also a correct result, but the minimum value of the parameter n is still equal to 30). With the double-precision format, the program falls into an infinite loop, that is, the result cannot be calculated.

If we calculate the specified example using the isclose function, then for the case of $rel_tol=1e-7$ for all formats of floating point numbers the result will be $n = 30$, $m = 15$, and for the value of the rel_tol parameter of greater precision (for example, already $rel_tol=1e-8$) – for float16, float64, float128, decimal.Decimal formats the result will be $n = 30$, $m = 15$, and for float32 format the result will still be $n = 35$, $m = 14$.

We can make an interesting intermediate conclusion: in some examples of computer calculations with floating point numbers, a given lower precision of calculations can give a more correct result than the procedure of increasing the precision. This effect is precisely what we observe in the described example: the correct answer is provided by the calculation with the float16 data type (as opposed to float32), the correct result is achieved with the value of the parameter $rel_tol=1e-7$, and not with the value $0 < rel_tol \leq 1e-8$.

Finally, we will consider the comparison of calculating the values of the square root of integers using two operations from the math module: sqrt and pow. Despite the simplicity of the problem statement, calculating the square root of a number, the whole root of a number, and especially the inverse square root of a natural number [29] is a relevant task both to correctness of calculations and the time efficiency of algorithms. For example, consider the range of numbers from 1 to 10000, the data type of floating point numbers is standard float (numpy.float64). We will iterate through the values until we find the number value such that $math.sqrt(number) \neq math.pow(number)$. Table 5 shows the following numbers (for example, less than 10000) depending on the version of Python and the compiler. The table shows only typical examples of the results of computer calculations of the proposed problem. For some

versions (for example, for Python 3.6.5 [GCC 7.3.1], there are no such values under the specified restrictions).

Table 5
Comparison of sqrt and pow functions

Python version	Compiler	Numbers		
3.7.4	GCC 9.2.0			
3.8.10	GCC 9.4.0			
3.9.9	GCC 11.1.0	2921,	3541,	5579,
3.10.6	GCC 11.3.0	7827,	8414,	8415
3.10.12	GCC 11.4.0			
3.11.5	GCC 13.2.1			
3.8.2	GCC 9.3.0	550,	971,	2921,
3.8.5	GCC 9.3.0	3541,	3543,	3884,
3.10.2	Clang 15.0.0	5579,	7827,	8414,
3.11.3	Clang 18.0.0	8415,	8451,	8800

Without going into the technical nuances of the implementation of these algorithms, I will explain the reason for the mismatch of values for the corresponding numbers from Table 5.

```

math.sqrt(2921) = 54.04627646748664204778833664022386074066162109375
binary(float64) 01000000 01001011 00000101 11101100
                 01100011 00100101 00110110 11111011

math.pow(2921, 0.5) = 54.04627646748663494236097903922200202941894531250
binary(float64) 01000000 01001011 00000101 11101100
                 01100011 00100101 00110110 11111010

```

We see from analysis of the binary representation of calculation results in float64 format that the difference is in the least significant bit of the mantissa. The reason is that the first discarded bit in the representation of the number is 1, and with the calculating `math.sqrt(2921)` this fact is taken into account. And 1 is added to the least significant bit of the mantissa, but not for calculating `math.pow(2921, 0.5)`. For example, both values are calculated with the increment of the least significant bit taken into account in Python 3.6.5 [GCC 7.3.1].

Conclusions

The work presents the results of the authors' research in the field of methodological foundations of teaching academic disciplines for students of the Computer Science specialty. The authors focused their attention on the topic of accuracy of computer calculations of various problems. This problem is relevant not only when performing engineering and scientific calculations, but also, as shown in the article, when solving the simple training problems. The authors focused on the study of the specified problem using the example of the numpy module, as one of the main software tools for modern scientific calculations.

The authors of the presented study focused on considering fairly simple examples of computer calculations that are completely correct from the point of view of the standards of computer work with numbers and arithmetic operations, the results are incorrect to a human performer. It has been demonstrated that mathematically correct calculations are often impossible to reproduce correctly within the IEEE-754 standard due to the fundamental limitations of the memory allocated to represent a specific number.

Using specific examples, it has been shown how the use of special Python computation features, such as the decimal module, can nevertheless lead to incorrect results. The use of external modules such as mpmath requires further research.

The work also gives paradoxical examples, when less accurate calculations allow you to get a more correct result. Such a statement contradicts the classical practices of calculation methods, and requires a more thorough study of the specifics of computer calculations.

It's important, for the training future specialists in the field of Computer Science during the teaching of subjects related to the accuracy of computer calculations and the fundamental limitations of computer calculations, to present all facts and principles from a single point of view so that students do not there was a false opinion about the arbitrariness of the results of computer calculations and the randomness of the corresponding errors of computer calculations. For a Computer Science professional, it is important not only to understand the basic principles of working with the floating-point number format from the standpoint of the generally accepted IEEE standard, but also to know, even at a basic level, possible modern alternatives, such as, for example, the concept of Posit.

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