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A COMPUTER HUNT FOR APERY'S CONSTANT

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1. INTRODUCTION

The zeta function $\zeta(z)$ given by the series (valid for $\mathrm{Re}(z) > 1$)

(1.1) $$\zeta(z) = \sum_{n=1}^{\infty} \frac{1}{n^z}$$

is one of the most important functions in mathematics. As early as 1734, Leonard Euler solved a long-standing problem by finding the "closed form" expression for $\zeta(2) = \frac{\pi^2}{6}$. The problem of finding $\zeta(2)$ had been worked on, without success, by many of the best mathematical minds of the time including John Wallis, John, James and Daniel Bernoulli, Christian Goldbach and Gottfried Wilhelm Leibniz. Not only did Euler find $\zeta(2)$, but he also showed that $\zeta(4) = \frac{\pi^4}{90}$, $\zeta(6) = \frac{\pi^6}{945}$, and in addition summed $\zeta(z)$ for every even positive integer z. (See the next section for more details.) Naturally Euler looked for a closed form for $\zeta(3)$ as well as $\zeta(z)$ when z is 5, 7, 9, …, but all such attempts failed. (See Ayoub [3] for an interesting historical summary of Euler's work on this and other topics.) To this day, we do not know if a nice closed form expression for these values of the zeta function exists. Only recently, Apery (see [1], [9] and [13]) proved that $\zeta(3)$ is irrational, and since then, $\zeta(3)$ has been known as "Apery's constant". It is not known if $\zeta(z)$ is irrational when z is 5, 7, 9, ….

In this paper we will hunt for a closed form expression for $\zeta(3)$ with the help of simple computer programs. Deep-sea divers who hunt for sunken treasure ships from Spanish galleons do not just dive anywhere in the wide ocean. They first look for old maps and other evidence that suggest where the ships perished. In the same way, we will seek evidence suggesting the probable appearance of the closed form for $\zeta(3)$. For example, the evidence listed above suggests that possibly $\zeta(3) = \frac{N}{D}\pi^3$, where N and D are natural numbers. Using a program like Mathematica we can get a numerical approximation to any desired precision like

$$\zeta(3) \approx 1.2020569031595942853938161511449990764986234 05.$$

We can let the computer try many values of N and D until we get very close to this number with $\frac{N}{D}\pi^3$. If we can repeat all 50 digits of the above approximation with relatively small values of N and D, we might have struck gold! We could then check more digits in the numerical expansion of Apery's constant. If the digits always checked exactly, our confidence would increase, but we would never be completely convinced of success. This is because we can never actually check all the digits. It would remain to prove mathematically that our result was correct, and the closed form we obtained might help in finding such a proof.

Most likely, our search will fail. However, even if we do not get the exact value of $\zeta(3)$, we will have obtained at least two items of information:

1. Our computer search would reveal that $\zeta(3)$ is *not* of a particular form for a given range of parameters. For example, if we search as above for the form $\frac{N}{D}\pi^3$, by allowing the computer to try all positive integer values of N and D less than 100,000, then we will be able to say that Apery's constant is *not* of this form for these values.
2. Our computer search will produce some values of the selected form that are very good *approximations* of Apery's constant. These simple approximations are sometimes of interest in themselves. For example, 22/7 and 355/113 are very good rational approximations for π that are frequently used.

2. THE EVIDENCE

There are infinitely many possible expressions that a "simple closed form" for Apery's constant $\zeta(3)$ might assume. For example, Apery proved that it is *not* of the form $\frac{N}{D}$, but it could take the form $\frac{N}{D}\pi^3$, or $\frac{N\sqrt{2}}{D}\pi^3$, or $\frac{N\sqrt{3}}{D}\pi^3$, or $\frac{N}{D}\pi^3+\frac{P}{Q}$, or $\frac{N}{D}\pi^3+\frac{P}{Q}\log 2$, …, (where N, D, P, and Q are integers). We begin by looking at known closed form expressions for series related to $\zeta(3)$.

Euler [7] found closed form expressions for $\zeta(z)$ when z is an even natural number. (See also Apostol [2], Berndt [5], Knopp [10] and Stark [14].) He showed that

$$\sum_{n=1}^{\infty}\frac{1}{n^2}=\frac{\pi^2}{6},$$

$$\sum_{n=1}^{\infty}\frac{1}{n^4}=\frac{\pi^4}{90},$$

$$\sum_{n=1}^{\infty}\frac{1}{n^6}=\frac{\pi^6}{945}\text{, and in general}$$

$$\sum_{n=1}^{\infty}\frac{1}{n^{2p}}=\frac{(-1)^{p+1}2^{2p-1}B_{2p}}{(2p)!}\pi^{2p}\ .$$

(See Knopp [10], page 237.) Here the numbers B_n are called Bernoulli's numbers, and they are all rational. The first few are

$$B_0=1, B_1=-\frac{1}{2}, B_2=\frac{1}{6}, B_4=-\frac{1}{30}, B_6=\frac{1}{42},\ldots\text{, and}\quad B_3=B_5=B_7=\ldots=0\,.$$

These can all be calculated recursively by starting with $B_0=1$, and using

$$\binom{n}{0}B_0+\binom{n}{1}B_1+\binom{n}{2}B_2+\cdots+\binom{n}{n-1}B_{n-1}=0$$

for $n=2,3,4,\cdots$.

Euler also found alternating series related to $\zeta(z)$. These include

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)^1}=\frac{\pi}{4},$$

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)^3}=\frac{\pi^3}{32},$$

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)^5}=\frac{\pi^5}{1536}\text{, and in general}$$

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)^{2p+1}}=\frac{(-1)^p E_{2p}}{2^{2p+2}(2p)!}\pi^{2p+1}\,.$$

(See Knopp [10], page 240.) Here the E_n are called Euler's numbers. They are all integers and the first few are $E_0=1, E_2=-1, E_4=5, E_6=-61, E_8=1385,\ldots$, and

$E_1 = E_3 = E_5 = ... = 0$. The E_{2n} can all be calculated recursively by starting with $E_0 = 1$, and then using

$$E_{2n} + \binom{2n}{2} E_{2n-2} + \binom{2n}{4} E_{2n-4} + \cdots + E_0 = 0 \text{, for } n = 1, 2, 3 \cdots .$$

Some of the series shown above suggest the possible closed form $\frac{N}{D}\pi^3$ for Apery's constant, but other series suggest more complex possibilities. For example, $\zeta(1)$ is undefined because the series $\sum_{n=1}^{\infty} \frac{1}{n^1}$ (harmonic series) diverges. However, the alternating series $\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^1} = \log 2$. Euler suggested that Apery's constant might involve $\log 2$, and this series might be the motivation for this idea.

A series of the form $\sum_{n=1}^{\infty} \frac{a_n}{n^z}$ is known as a Dirichlet series. (See Edwards [6], and Titchmarsh [15].) Examples of other Dirichlet series of interest include those given recently by Balanzario [4]. These series are periodic in the sense that the given numerators repeat. Below are three such series:

$$\frac{1}{1^5} + \frac{0}{2^5} + \frac{-1}{3^5} + \frac{0}{4^5} + \cdots = \frac{5\pi^5}{1536} \text{, (period 4),}$$

$$\frac{1}{1^3} + \frac{1}{2^3} + \frac{-1}{3^3} + \frac{-1}{4^3} + \frac{0}{5^3} + \cdots = \frac{4\pi^3}{625}\sqrt{25 + 2\sqrt{5}} \text{, (period 5), and}$$

$$\frac{1}{1^3} + \frac{0}{2^3} + \frac{1}{3^3} + \frac{0}{4^3} - \frac{1}{5^3} + \frac{0}{6^3} - \frac{1}{7^3} + \frac{0}{8^3} \cdots = \frac{3\pi^3}{64\sqrt{2}} \text{. (period 8).}$$

For example, in the first series the sequence of numerators 1, 0, -1, 0 is shown, so they are to be repeated again and again yielding

$$\sum_{n=0}^{\infty}\frac{1}{(4n+1)^5}+\frac{0}{(4n+2)^5}+\frac{-1}{(4n+3)^5}+\frac{0}{(4n+4)^5}=\frac{5\pi^5}{1536}.$$

From the evidence gathered above, we conclude that our computer search can begin profitably by examining the following possible expressions for Apery's constant:

$$\frac{N}{D}\pi^3,\ \frac{N\sqrt{2}}{D}\pi^3,\ \frac{N\sqrt{3}}{D}\pi^3,\ \frac{N}{D}\log 2\ ,\ \frac{N}{D}\sqrt{3}\log 2 \text{ and } \frac{N}{D}\pi^3\log 2\,.$$

where *N* and *D* are natural numbers. We also notice that the numbers *N* and *D* are likely to be small, say under 500, based on the integers that are shown in specific closed form expressions above. Many other possible closed forms are of interest, but we will concentrate on the above simple forms in this paper.

3. GOOD RATIONAL APPROXIMATIONS

Suppose we are testing the possible closed form expression $\frac{N}{D}\pi^3$ for $\zeta(3)$. Our computer search will then try to identify rational numbers $\frac{N}{D}$, which are very close to $\frac{\zeta(3)}{\pi^3}$. This raises the question of "what is close"? By taking the denominator *D* to be large enough, we can get as close as we like. But how close can we get if the denominator is not large? In more precise terms, if a real number *x* and the denominator *D* are given, how close can we expect the rational number $\frac{N}{D}$ to be to *x*? How small can we expect the error $\left|\frac{N}{D}-x\right|$ to be? A little thought shows that we can always find *N* so that $\left|\frac{N}{D}-x\right|\le\frac{1}{2D}$. But can we do better? The theory of continued fractions, outlined in the appendix reveals that if we let D vary over all the positive integers, then for an irrational number x there are infinitely many values of D such that

$$\left|\frac{N}{D} - x\right| < \frac{1}{2D^2}.$$

If x is rational, only a finite number of such fractions exist. We will call rational approximations "good" if they satisfy this last inequality.

4. A COMPUTER SEARCH

As in most mathematical problems, in this instance, there are several ways to solve our problem. We will look at the simplest approach first. In our case, we are using a computer program to find a closed form expression of $\zeta(3)$. The following is pseudo-code for a scan for possible integers for the form $\frac{N}{D}\pi^3$:

```
10    Max = 1000            // Max is the largest value of N and D that will be scanned
20    D = 1                 // Starts the denominator at 1
30    While ( D <= Max ,    // Begin scan of denominator
40          N=1             // Sets the numerator to 1
50          While ( N <= Max,     // begin scan of numerator at given denominator
60                Error = 1 / 2D^2   // a "good" error
70                If ( |ζ(3)/π^3 − N/D| ≤ Error )  Output Values of N and D
80                N = N + 1       // increments N
90          )                     // end of loop for the numerator
100         D = D + 1       // increment D
110   )                     // end of loop for denominator
```

This program will scan all combinations of the numerator and denominator up to values of 1000 and outputs the combinations that are within a given margin of error. The program can be adjusted in Line 70 to fit any of the possible forms for $\zeta(3)$ that are to be tested.

This is a rather tedious method but the easiest to understand. More advanced algorithms that can be used include continued fractions. The following is a table of small number fractions that can be used to approximate each possible form of $\zeta(3)$, along with its absolute error and its error in terms of $1/2D^2$. The absolute error is given by $\left|\zeta(3)-\frac{N}{D}\pi^3\right|$ for the case where we assume $\zeta(3)=\frac{N}{D}\pi^3$. The second form of error gives us an idea of how good the approximation is relative the size of the denominator and is determined by $\left|\frac{\zeta(3)}{\pi^3}-\frac{N}{D}\right|(2D^2)$. It should be noted that no exact match was found.

Table 1: Approximations of $\zeta(3)$

Form of $\zeta(3)$	Close Fraction	Absolute Error	Error in Terms of $1/2D^2$
$\frac{N}{D}$	$\frac{119}{99}$	$3.6*10^{-5}$	0.7194
$\frac{N}{D}\pi^3$	$\frac{5}{129}\pi^3$	$2.6*10^{-4}$	0.2824
$\frac{N}{D}\sqrt{2}\pi^3$	$\frac{2}{73}\sqrt{2}\pi^3$	$1.5*10^{-5}$	0.1702
$\frac{N}{D}\sqrt{3}\pi^3$	$\frac{3}{134}\sqrt{3}\pi^3$	$2.8*10^{-4}$	0.1872
$\frac{N}{D}\log 2$	$\frac{137}{79}\log 2$	$1.6*10^{-5}$	0.3034

$\frac{N}{D}\sqrt{3}\log 2$	$\frac{806}{805}\sqrt{3}\log 2$	$6.2*10^{-7}$	0.6693
$\frac{N}{D}\pi^3\log 2$	$\frac{8}{143}\pi^3\log 2$	$2.8*10^{-4}$	0.5478

Using QUICK BASIC we were able to determine that no values of the denominator less than 10^{15} will work for any of the above forms. With the help of Mathematica, it appears that no values for the denominator less that 10^{50} will work for any of the above forms and that the denominator must be larger than a googol, 10^{100}, for simplest form, $\frac{N}{D}\pi^3$, to work. In this case, we find that

$$\frac{52785569273392031249497640694293062133207508234671839926997230937616654007259447450068939952876428475650298}{13615694575821818287635241279024527831175005343255284610276129037594485666212441547579585847967964720713 83357}\pi^3$$

approximates $\zeta(3)$ to within an absolute error of 10^{-215} and the denominator is on the order of 10^{108}.

5. FINAL REMARKS

It is interesting to see that our computer search for a closed form for Apery's constant is closely related to the subject of simple continued fractions. For this reason we have included an appendix to this paper which outlines the ideas from the theory of continued fractions which are applicable here. Our previous program, when searching for rational approximations to the number $\frac{\zeta(3)}{\pi^3} = 0.0387681796029168\cdots$, found the following sequence of numbers:

$$\frac{1}{26}, \frac{5}{129}, \frac{34}{877}, \frac{107}{2760}, \frac{141}{3637}, \frac{248}{6397}, \frac{885}{22828}, \frac{9487}{244711}, \dots .$$

When the same number is expanded in a continued fraction we get

$$\frac{\zeta(3)}{\pi^3} = [0; 25, 1, 3, 1, 6, 3, 1, 1, 2, 1, 10, 3, 2, 1, \ldots].$$

(See the Appendix for a definition of this list notation.) This continued fraction generates the sequence of convergents:

$$\frac{1}{25}, \frac{1}{26}, \frac{4}{103}, \frac{5}{129}, \frac{34}{877}, \frac{107}{2760}, \frac{141}{3637}, \frac{248}{6397}, \frac{637}{16431}, \frac{885}{22828}, \frac{9487}{244711}, \ldots .$$

Notice that the previous sequence is a subsequence of the above.

We have only begun to explore possible closed forms for Apery's constant. The reader might want to continue the search.

APPENDIX ON SIMPLE CONTINUED FRACTIONS

In this appendix we list ideas from the theory of continued fractions that are directly related to our search for a closed form for $\zeta(3)$.

Suppose we try to find simple fractions (rational approximations) which are close to the number $\pi \approx 3.141592654$. Consider the following simple steps performed using a calculator:

$$3.141592654 = 3 + 0.141592654$$

$$= 3 + \frac{1}{\frac{1}{0.141592654}}$$

$$= 3 + \frac{1}{7.062513306}$$

This gives us the simple approximation $\pi \approx 3 + \frac{1}{7} = \frac{22}{7}$. Next we repeat the above calculations with the number 7.062513306 and get:

$$3.141592654 = 3 + \frac{1}{7 + 0.062513306}$$

$$= 3 + \cfrac{1}{7 + \cfrac{1}{\cfrac{1}{0.062513306}}}$$

$$= 3 + \cfrac{1}{7 + \cfrac{1}{15.99659428}}$$

This last expression suggests the approximation $3 + \cfrac{1}{7 + \cfrac{1}{15}} = \frac{333}{106}$. Continuing the calculation we get

$$3.141592654 = 3 + \cfrac{1}{7 + \cfrac{1}{15 + 0.99659428}}$$

$$= 3 + \cfrac{1}{7 + \cfrac{1}{15 + \cfrac{1}{\cfrac{1}{0.99659428}}}}$$

$$= 3 + \cfrac{1}{7 + \cfrac{1}{15 + \cfrac{1}{1.003417359}}}$$

This last expression suggests the approximation $3 + \cfrac{1}{7 + \cfrac{1}{15 + \cfrac{1}{1}}} = \frac{355}{113}$.

We call the expression $3+\cfrac{1}{7+\cfrac{1}{15+\cfrac{1}{1}}}$ a *simple continued fraction* or just a *continued fraction.* Since it is awkward to write this expression, we sometimes use the notation $3+\frac{1}{7+}\ \frac{1}{15+}\ \frac{1}{1}$ or the list notation [3; 7, 15, 1] The numbers 3, 7, 15,1 are called *partial quotients*, and the rational approximations 3, 22/7, 333/106 and 355/113 are called *convergents.* Of course, we can continue the calculation and get more rational approximations to π. In general, a simple continued fraction can be described in the list notation by $[a_0; a_1, a_2, a_3, \cdots]$, where $a_1, a_2, a_3, \cdots$ are all positive integers. Continuing the computations for π we get

$$\pi = [3; 7, 15, 1, 292, 1, 1, 1, 2, 1, 3, 1, 14, 2, 1, 1, 2, 2, 2, 2, 1, 84, 2, \ldots].$$

There does not seem to be any recognizable regularity in this sequence.

In the following, we will state theorems about continued fractions, without proof. Detailed proofs can be found in Hardy and Wright [8]. Other good books on continued fractions include Moore [11] and Olds [12].

Let *x* be any given real number, and let its simple continued fraction, calculated by the procedure given above be $x=[a_0; a_1, a_2, a_3, \cdots]$, where $a_1, a_2, a_3, \cdots$ are all positive integers. Let the convergents be denoted by $\frac{p_0}{q_0}, \frac{p_1}{q_1}, \frac{p_2}{q_2}, \cdots$. It is easy to see that $\frac{p_0}{q_0}=\frac{a_0}{1}$, $\frac{p_1}{q_1}=\frac{a_0a_1+1}{a_1}$, … . To find the remaining convergents it is convenient to use the recursion relations given by the following theorem:

Theorem 1: (See [8], Theorem. 149, page 130.)

For $n = 2, 3, 4, \cdots$ *we have* $p_n = a_n p_{n-1} + p_{n-2}$ *and* $q_n = a_n q_{n-1} + q_{n-2}$.

We illustrate the calculation of p_n and q_n by using a table. For the number π studied above we would write

n	0	1	2	3	4	5
a_n	3	7	15	1	292	1
p_n						
q_n						

Next we use the easy expressions $\frac{p_0}{q_0} = \frac{a_0}{1}$, $\frac{p_1}{q_1} = \frac{a_0 a_1 + 1}{a_1}$, to complete the entries for *n* = 0,1.

n	0	1	2	3	4	5
a_n	3	7	15	1	292	1
p_n	3	22				
q_n	1	7				

To find p_2 we use the relation $p_2 = a_2 p_1 + p_0 = 15 \bullet 22 + 3 = 333$. In a similar way we get $q_2 = a_2 q_1 + q_0 = 15 \bullet 27 + 1 = 106$

n	0	1	2	3	4	5
a_n	3	7	15	1	292	1
p_n	3	22	333			
q_n	1	7	106			

In a similar way the remaining entries are filled in, column by column:

n	0	1	2	3	4	5
a_n	3	7	15	1	292	1
p_n	3	22	333	355	103993	104348
q_n	1	7	106	115	33102	33215

Theorem 2: (See [8], Theorems 152, 153 and 159.)

The even convergents, $\frac{p_0}{q_0}, \frac{p_2}{q_2}, \frac{p_4}{q_4}, \cdots,$ *form a monotonically increasing sequence, while the odd convergence form a monotonically decreasing sequence. Both sequences converge to x.*

The decimal representation of a rational number is sometimes terminating and sometimes infinite and repeating. The next theorem tells us a similar criteria for simple continued fractions.

Theorem 3: (See [8], Theorems 158 to 170, pages 133 to 140.)

If x is irrational, then its expansion as a simple continued fraction, $x = [a_0; a_1, a_2, \cdots]$*, is infinite and unique. If x is rational, then its simple continued fraction is finite and unique except for the last partial quotient since* $x = [a_0; a_1, a_2, \cdots, a_n] = [a_0; a_1, a_2, \cdots, a_n - 1, 1]$.

The following two theorems tell us that the partial quotients $\frac{p_n}{q_n}$ are always good rational approximations.

Theorem 4: (See [8], Theorem. 171, page 140.)

For all $n = 1, 2, 3, \cdots$ *we have* $\left|\frac{p_n}{q_n} - x\right| < \frac{1}{q_n{}^2}$.

Theorem 5: (See [8], Theorem. 183, page 152.)

Given two consecutive convergents, at least one of them satisfies

$$\left|\frac{p_n}{q_n} - x\right| < \frac{1}{2{q_n}^2}.$$

The next theorem tells us that all "good rational approximations" are convergents of the simple continued fraction.

Theorem 6: (See [8], Theorem. 184, page 153.)

If the fraction $\frac{p}{q}$ *satisfies* $\left|\frac{p}{q} - x\right| < \frac{1}{2q^2}$, *then* $\frac{p}{q}$ *is one of the convergents*

$\frac{p_0}{q_0}, \frac{p_1}{q_1}, \frac{p_2}{q_2}, \cdots$, *of the simple continued fraction for x.*

The next theorem tells us that the convergents are always completely reduced fractions.

Theorem 7: (See [8], Theorem. 157, page 132.)

If $\frac{p_n}{q_n}$ *is a convergent of the simple continued fraction for x, then* p_n *and* q_n *have no common factor.*

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