

Continued Fractions, Algebraic Numbers and Modular Invariants

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Brillhart discovered in 1965 that the continued fraction of the real root of the cubic equation $x^3 - 8x - 10 = 0$ has a number of very large partial quotients. In this paper we explain why this phenomenon is surprising and then show how its consideration naturally leads one into some very deep branches of the theory of numbers before the reason for the phenomenon becomes clear. In order to make the paper intelligible to non-specialists we give a brief account of the classical theories of continued fractions, quadratic forms and modular functions in the appropriate sections.

1. Introduction

DURING A VISIT to San Francisco in June 1965 one of us (R.F.C.) was told by D. H. Lehmer that John Brillhart had been using their computer to study the continued fraction expansions of certain algebraic numbers of the third and fourth degrees. Some years earlier Delone & Faddeev (1964) had made a similar study of the roots of cubic equations of the type

$$x^3 - ax - b = 0 \tag{1}$$

where a, b are integers and $|a|, |b| \leq 9$. They had found no results of any interest. Brillhart, having access to an IBM 7094, had decided to extend the range of search and almost immediately he found something which the Russians had narrowly missed. One of the several thousand numbers studied had produced results of unusual interest in that among the first 200 partial quotients there was one greater than 16,000,000 and seven others greater than 20,000. The number in question is the real root of $x^3 - 8x - 10 = 0$. The discriminant of the cubic equation (1) is $4a^3 - 27b^2$ and so the discriminant of $x^3 - 8x - 10$ is $-652 = 4 \times (-163)$. Now the number -163 appears in a significant role in algebraic number theory (as will be explained in Section 3, below) and the question Lehmer posed was whether this apparent connection is real or not. If it is real can one predict other algebraic equations whose roots also have unusual continued fractions?

Some months later we were able to repeat Brillhart's calculation of the root of this cubic to several hundred places of decimals and obtained complete agreement. We were able to do this by using a very fine multi-length arithmetic package for Atlas written by W. F. Lunnon of Manchester University. The value of the root, to 200 places, and the first 200 partial quotients of its continued fraction are given in Table 1. The computing time required to do this on Atlas was only ten seconds. Confident that we now had a sufficiently powerful programming package available we set about

trying to explain the phenomenon. The explanation is given in Section 5. The next three sections provide the necessary background information.

2. Continued Fractions

Let θ be any positive real number. Let

$$a_0 = [\theta], \quad r_0 = (\theta - a_0)^{-1}$$

where, as usual, $[x]$ denotes the integral part of x . Define, for $n \geq 0$

$$a_{n+1} = [r_n], \quad r_{n+1} = (r_n - a_{n+1})^{-1}.$$

Then we say that θ has the continued fraction representation

$$\theta = a_0 + \frac{1}{a_1 + \frac{1}{a_2 + \frac{1}{a_3 + \dots}}} \quad (2)$$

and the elements a_i are called "the partial quotients" of the continued fraction. It is well known that the continued fraction for θ terminates if and only if θ is rational and that the continued fraction is periodic if and only if θ is a quadratic irrational. For example

$$\frac{7}{5} = 1 + \frac{2}{5} = 1 + \frac{1}{2\frac{1}{2}} = 1 + \frac{1}{2 + \frac{1}{2}};$$

whereas

$$\sqrt{2} = 1 + \frac{1}{2 + \frac{1}{2 + \frac{1}{2 + \dots}}}.$$

It is natural to ask if the continued fractions of the roots of cubic (or higher degree) equations have any properties; for example:

Problem 1. If θ in (2) satisfies a cubic equation, are the a_i bounded?

The answer is not known. We might also ask how many of the a_i we might expect to have a particular numerical value, such as 17. In this case there is a theorem, first stated by Gauss in a letter to Laplace but the first published proof of which, due to Kusmin, did not appear until 1928. This theorem tells us something about the probability distribution of the a_i for *almost all* real numbers; it can be stated:

THEOREM. Let θ be a real number in $(0, 1)$ and suppose

$$\theta = \frac{1}{a_1 + \frac{1}{a_2 + \frac{1}{a_3 + \dots}}},$$

then, for almost all θ

$$\text{prob}(a_i = k) = \log_2 \frac{(k+1)^2}{k(k+2)}.$$

For a proof of this see the book by Khinchin (1963: 81). Thus, for almost all real numbers, we expect about 41% of the a_i to have the value 1, 17% to be 2 and so on. Unfortunately since the theorem refers only to "almost all θ " and since the field of algebraic numbers has measure zero it is possible that the theorem does not apply to any algebraic numbers at all. We note that it does not apply to *any* algebraic numbers of degree one to two. Without much hope of an answer we therefore ask:

Problem 2. Does the distribution of the partial quotients of a continued fraction of a cubic irrational follow Gauss' Law as given in the above theorem?

It should by now be clear that anything which throws light on the continued fractions of cubic irrationals is likely to arouse interest, for the theoretical analysis of the problem is formidable. This accounts for the calculations of Delone & Faddeev and the more recent work of Brillhart as well as several other people. When people compute continued fractions to a large number of terms what do they look for? Hopefully, something unusual; too many or too few terms having the value 1 or too many "large" terms, for example. The theorem above gives us some idea of how "large" a term we might expect to find if we compute a continued fraction to, say, N terms. For

$$\text{prob}(a_i = k) = \log_2 \frac{(k+1)^2}{k(k+2)}$$

and so

$$\text{prob}(a_i \geq k) = \sum_{m=k}^{\infty} \log_2 \frac{(m+1)^2}{m(m+2)} = \log_2 \left(1 + \frac{1}{k}\right) \sim \frac{1.44}{k}. \quad (3)$$

Thus the probability that *any particular* partial quotient has a value greater than 1000 is about $1/690$ and so, if we compute the continued fraction to 200 terms we shall be lucky if we find one such case. Now Brillhart computed approximately 200 terms of "several thousand" continued fractions. If we say 5000 this means he computed 1,000,000 partial quotients. Hence, from (3), he might have expected to find one or two partial quotients which exceeded 1,000,000. What he did not expect to find was one term greater than 16,000,000 and one term of more than 1,500,000 in the expansion of *the same algebraic number*. When it is then found that this number also produces a term greater than 300,000 and several other "large" terms interest is naturally aroused.

3. Binary Quadratic Forms. Class Number

Given rational integers a, b, c we define a binary quadratic form (a, b, c) by

$$f(x, y) = ax^2 + bxy + cy^2,$$

and we call the number $b^2 - 4ac$ "the discriminant of $f(x, y)$ ". If we make a substitution $x = \alpha u + \beta v$, $y = \gamma u + \delta v$, $f(x, y)$ is transformed into a form $g(u, v)$ and the discriminant of $g(u, v)$ will be found to be

$$(b^2 - 4ac)(\alpha\delta - \beta\gamma)^2. \quad (4)$$

Denote the coefficients of $g(u, v)$ by a', b', c' . If $\alpha, \beta, \gamma, \delta$ are rational integers and $(\alpha\delta - \beta\gamma) = 1$, in which case the substitution is called "unimodular", we see from (4) that $f(x, y)$ and $g(u, v)$ have the same discriminant. We then say that the forms (a, b, c) and (a', b', c') are "equivalent" and we write $(a, b, c) \sim (a', b', c')$. Thus for example the form

$$f(x, y) = x^2 + 3y^2$$

is transformed into

$$g(u, v) = 31u^2 + 40uv + 13v^2$$

by the unimodular transformation $x = 2u + v$, $y = 3u + 2v$ and f and g will both be found to have discriminant -12 .

Two binary quadratic forms which are equivalent necessarily have the same discriminant. Is the converse true; i.e. if two forms f, g have the same discriminant can we be sure that there exists an integral unimodular transformation which carries f into g ? The answer is "no". For example the two forms x^2+5y^2 and $2x^2+2xy+3y^2$ both have discriminant -20 but it can easily be proved that they are not equivalent. On the other hand it can also be proved that any binary quadratic form of discriminant -20 is equivalent to one of these two forms.

This last result is a particular case of the following theorem

THEOREM. *Let D be given. If $f(x, y) = ax^2 + bxy + cy^2$ is a binary quadratic form of discriminant $D = b^2 - 4ac$, then f is equivalent to one of a finite set of forms.*

The number of forms in this finite set depends upon the value of D . It is denoted by $h(D)$ and called "the class number of the discriminant D ". A particular importance is attached to those values of D for which $h(D) = 1$ for in this case all forms of the given discriminant are equivalent to a single form and it can be shown that this implies that the integers of the algebraic number field $k(\sqrt{D})$, obtained by adjoining \sqrt{D} to the rationals, possess the property of unique factorization. When $D < 0$ the only values of D for which $h(D) = 1$ are given by

$$-D = 3, 4, 7, 8, 11, 19, 43, 67, 163.$$

Although it had been suspected for many years that $D = -163$ is the last negative discriminant associated with class number 1 it is only recently that this has been definitely established (Stark, 1967).

We therefore see why the number -163 appearing as the discriminant of a quadratic equation is of interest to a number theorist. However, the equation in which we are interested is a *cubic* and its discriminant is $4 \times (-163)$. The factor 4, being a square, is of little importance in the theory of quadratic forms and can be ignored. The former point turns out to be the key to the whole business as will be shown in the next section.

4. Modular Functions and Klein's Modular Invariant

The Weierstrass elliptic function, $\wp(z)$, is defined as

$$\wp(z) = \frac{1}{z^2} + \sum'_{m,n} \left\{ \frac{1}{(z-\Omega)^2} - \frac{1}{\Omega^2} \right\}$$

where $\Omega = 2m\omega_1 + 2n\omega_2$, the numbers ω_1, ω_2 being complex and the ratio ω_1/ω_2 not purely real; the ' on the summation sign denoting, as usual, that the term $m = n = 0$ is excluded. It is easy to see that $\wp(z)$ satisfies the differential equation

$$\wp'(z)^2 = 4\wp^3(z) - g_2\wp(z) - g_3, \tag{5}$$

where $g_2 = 60 \sum' \Omega^{-4}$ and $g_3 = 140 \sum' \Omega^{-6}$. The roots of the cubic (5) can be shown to be

$$\wp\left(\frac{\omega_1}{2}\right), \quad \wp\left(\frac{\omega_2}{2}\right), \quad \wp\left(\frac{\omega_1 + \omega_2}{2}\right),$$

and these are all different, hence the discriminant of the cubic

$$\Delta(\omega_1, \omega_2) = g_2^3 - 27g_3^2 \neq 0.$$

If we divide out by the appropriate powers of ω_1 and put $\tau = \omega_2/\omega_1$ we deduce that

$$\begin{aligned} g_2 &= \omega_1^{-4}g_2(1, \tau), \\ g_3 &= \omega_1^{-6}g_3(1, \tau), \\ \Delta &= \omega_1^{-12}\Delta(1, \tau), \end{aligned}$$

and hence the ratio

$$J(\tau) = \frac{g_2^3}{\Delta} = \frac{g_2^3(1, \tau)}{\Delta(1, \tau)}$$

depends only on the ratio, τ , of ω_2 to ω_1 .

If a, b, c, d are integers and $ad - bc = 1$ then a \wp function based on the periods $\omega'_1 = a\omega_1 + b\omega_2$ and $\omega'_2 = c\omega_1 + d\omega_2$ will be the same as the original \wp function based on ω_1 and ω_2 . Hence g_2, g_3 and so Δ will be unchanged and so $J(\tau)$ will also be unchanged; thus $J(\tau)$ will have the property that

$$J(\tau) = J\left(\frac{a\tau + b}{c\tau + d}\right) \text{ for } ad - bc = 1$$

so that $J(\tau)$ is an elliptic modular function.

Let $q = e^{\pi i \tau}$. Then it can be shown (Weber, 1908: 179) that

$$1728J(\tau) = j(\tau) = \left[\frac{f^{24}(\tau) - 16}{f^8(\tau)} \right]^3, \tag{6}$$

where

$$f(\tau) = q^{-1/24} \prod_{n=1}^{\infty} (1 + q^{2n-1}). \tag{7}$$

The function $j(\tau)$ is called ‘‘Klein’s modular invariant’’. It is known (Lehmer, 1942: 488) that

$$j(\tau) = q^{-2} + 744 + 196884q^2 + 21493760q^4 + \dots \tag{8}$$

the coefficients being integral. Furthermore if $d > 0$ is a prime and $h(-d) = 1$ then $j\left(\frac{-1 + \sqrt{-d}}{2}\right)$ is itself an integer (indeed it is a perfect cube). Denoting this integer by N and observing that

$$q^2 = \exp(2\pi i \tau) = -e^{-\pi \sqrt{d}}$$

we find that

$$e^{\pi \sqrt{d}} = -N + 744 - 196884 e^{-\pi \sqrt{d}} + 21493760 e^{-2\pi \sqrt{d}} - \dots \tag{9}$$

It is known (Lehmer, 1942: 488) that the coefficients of the powers of $e^{-\pi \sqrt{d}}$ are heavily outweighed by these negative exponentials so that if d is large it follows from (9) that $e^{\pi \sqrt{d}}$ must be very close to an integer, the error being approximately $-196884 e^{-\pi \sqrt{d}}$.

We have seen that the last value of d for which $h(-d) = 1$ is $d = 163$ and computation shows that in this case

$$e^{\pi \sqrt{163}} = 262537412640768743.999999999999250\dots \tag{10}$$

We now show that $e^{2\pi \sqrt{163}}$ must also be very close to an integer (which is not obvious).

Let $M = -N + 744$ in (9). Then if $x = e^{\pi \sqrt{163}}$

$$x = M - 196884x^{-1} + 21493760x^{-2} - \dots$$

so that

$$\begin{aligned}
 x^2 &= Mx - 196884 + 21493760x^{-1} \dots \\
 &= M(M - 196884x^{-1} + 21493760x^{-2} \dots) - 196884 + 21493760x^{-1} - \dots \\
 &= M^2 + M(-196884x^{-1} + 21493760x^{-2} \dots) - 196884 + 21493760x^{-1} - \dots \\
 &= M^2 + (x + 196884x^{-1} - 21493760x^{-2} \dots)(-196884x^{-1} + 21493760x^{-2} - \dots) - \\
 &\hspace{15em} 196884 + 21493760x^{-1} - \dots \\
 &= M^2 - 393768 + 42987520x^{-1} + 0(x^{-2}). \tag{11}
 \end{aligned}$$

The value of x is given by (10) and we therefore deduce that $x = e^{2\pi\sqrt{163}}$ should differ from an integer by approximately $42987520/262537412640768744 \doteq 1.63739 \times 10^{-10}$, the error being one of excess.

In a similar manner one could deal with $e^{3\pi\sqrt{163}}$, $e^{4\pi\sqrt{163}}$. It is found that the first seven powers of $e^{\pi\sqrt{163}}$ are close to integers, the error increasing fairly rapidly. The fractional parts of the powers of $x (= e^{\pi\sqrt{163}})$ are shown below.

Power of x	Fractional part
x	.99999999999250
x^2	.000000000163738
x^3	.999999990123693
x^4	.000000308464322
x^5	.999993654187468
x^6	.000097175254162
x^7	.998809316526134

4.1. *Class Invariants*

We have already remarked that if $d > 0$ is a prime and $h(-d) = 1$ then $j\left(\frac{-1+\sqrt{-d}}{2}\right)$ is itself an integer. From (6) this shows that $f\left(\frac{-1+\sqrt{-d}}{2}\right)$ satisfies an algebraic equation. Since $j(\tau)$ is a modular function, $j(\tau + 1) = j(\tau)$ and so

$$j\left(\frac{-1+\sqrt{-d}}{2}\right) = j\left(\frac{1+\sqrt{-d}}{2}\right)$$

and this implies that $f\left(\frac{1+\sqrt{-d}}{2}\right)$ is algebraic also. Furthermore it is easy to see from (7), that

$$f^{24}\left(\frac{1+\sqrt{-d}}{2}\right)f^{24}\left(\frac{-1+\sqrt{-d}}{2}\right) = f^{24}(\sqrt{-d})$$

and so $f(\sqrt{-d})$ is also algebraic whenever $h(-d) = 1$. It is in fact true that, even if $h(-d) > 1$, $f(\sqrt{-d})$ still satisfies an algebraic equation but the degree of the equation depends upon the value of $h(-d)$. The theory of these class invariants, as they are known, is given in detail in Weber (1908) and a table is provided on pages 721-726 showing the algebraic equations satisfied by $f(\tau)$ for a large number of values of d up to $d = 193$ and for a few more values up to $d = 1848$. Thus, corresponding to $d = 1$ we find $f^{24}(i) = 64$, that is

$$e^{\pi} \prod_{n=1}^{\infty} (1 + e^{-(2n-1)\pi})^{24} = 64,$$

and again corresponding to $d = 3, f^{24}(i\sqrt{3})$, i.e.

$$e^{\pi\sqrt{3}} \prod_{n=1}^{\infty} (1 + e^{-(2n-1)\pi\sqrt{3}})^{24} = 256.$$

A more comprehensive list is given by Watson (1936). Corresponding to the case $d = 163$ we have

$$f(i\sqrt{163}) = x$$

where

$$x^3 - 6x^2 + 4x - 2 = 0. \tag{12}$$

If we write $x = z + 2$ in (12) it reduces to

$$z^3 - 8z - 10 = 0 \tag{13}$$

which is Brillhart's cubic! Now

$$f(i\sqrt{163}) = e^{\pi\sqrt{163}/24} \prod_{n=1}^{\infty} (1 + e^{-(2n-1)\pi\sqrt{163}}). \tag{14}$$

The value of this expression is dominated by the factor $e^{\pi\sqrt{163}/24}$ the remaining factors tending to unity with great rapidity. The largest is the first which, from (10), is about $1 + 4 \times 10^{-18}$. We see therefore that we have established the following:

THEOREM. *If x denotes the real root of the equation $x^3 - 8x - 10 = 0$ then $x + 2$ has the value given by the right-hand side of (14), and, within an error of less than 10^{-17}*

$$x + 2 \doteq e^{\pi\sqrt{163}/24}. \tag{15}$$

4.2. The Pseudo Class Invariant

We now have all the information necessary to dispose of the problem which we stated in the introduction. We know that the root of Brillhart's cubic, x , has a remarkable continued fraction and we now know that $(x + 2)$ is given accurately by (14) and to 17 places of decimals by (15). We therefore computed the continued fraction of $e^{\pi\sqrt{163}/24}$ and we found that not only was this continued fraction quite unremarkable but the values of the partial quotients first differ from the partial quotients of $x + 2$ at the 16th term, which is immediately before the first large term (22,986) occurs. This implies that the first factor ignored, viz.

$$1 + e^{-\pi\sqrt{163}}$$

is, in some sense, responsible for the first large term in the continued fraction for $x + 2$. Now we have seen, (10), that $e^{\pi\sqrt{163}}$ is very nearly an integer, the error being negative, and so

$$1 + e^{-\pi\sqrt{163}} = 1 + \frac{1}{M_1 + 1} \frac{1}{1 + N_1 +}$$

where $M_1 = 262537412640768743$ and $N_1 = 1333462407511$. The second factor ignored is $1 + e^{-3\pi\sqrt{163}}$ and this is also close to an integer, the error also being on the negative side, so that

$$1 + e^{-3\pi\sqrt{163}} = 1 + \frac{1}{M_2 + 1} \frac{1}{1 + N_2 +} \dots$$

where $M_2 \doteq 1.8 \times 10^{52}$ and $N_2 \doteq 10^8$.

Similar remarks apply to the third and fourth factors, the corresponding values of M_i, N_i being about

$$\begin{aligned} M_3 &\doteq 1.24 \times 10^{87}, & M_4 &\doteq 8.6 \times 10^{121}, \\ N_3 &\doteq 1.56 \times 10^5, & N_4 &\doteq 800. \end{aligned}$$

Some further calculations led us to the conclusion that the very large terms in Brillhart's continued fraction are caused by the presence of these unusual factors which contain two large integer terms separated by a single 1. In order to test this hypothesis we computed the continued fraction obtained by taking N_1, N_2, N_3, N_4 to be infinite. This is achieved in practice by replacing (14) by

$$f_1(u) = u^{1/24}(1+z_1^{-1})(1+z_3^{-1})(1+z_5^{-1})(1+z_7^{-1}) \dots \tag{16}$$

where $u = e^{\pi\sqrt{163}}$ and $z_n = [u^n + \frac{1}{2}]$, so that z_n is the integer nearest to u^n . The value $f_1(u)$ so obtained is of course extremely close to that obtained from (14), the error being only about 5.8×10^{-47} . Despite this minute numerical change the effect on the continued fraction is catastrophic. Only the first large term (22986) remains, the others have completely disappeared. When the factors in (16) are replaced, one by one, by their correct values the large partial quotients reappear one or two at a time.

The value of (16), which we called "the pseudo class invariant", and the expansion of its continued fraction are given in Table 2.

5. Conclusions

The numerical evidence shows that the reasons why the root of the cubic $x^3 - 8x - 10 = 0$ has a remarkable continued fraction are:

- (i) the equation is, effectively, the equation of the class invariant associated with discriminant -163 ;
- (ii) the algebraic number field $k(\sqrt{-163})$ has class number 1;
- (iii) the root x of the equation is approximated to seventeen places of decimals by $x' = -2 + e^{\pi\sqrt{163}/24}$;
- (iv) the ratio x/x' is given by the product

$$\prod_{n=1}^{\infty} (1 + e^{-(2n-1)\pi\sqrt{163}});$$

- (v) the first few terms of this product can all be written in the form

$$1 + \frac{1}{M_i + 1} \frac{1}{1 + N_i} \dots$$

where M_i is "very large" and N_i is "large";

- (vi) the presence of such factors as these produces large terms in the continued fraction expansion for x . When these factors are replaced by $1 + (1/M_i + 1)$ the large terms disappear although the resulting change in the value of x is extremely small.

On the basis of these observations we can therefore make some predictions. We have seen that $e^{\pi\sqrt{163}}$ is very nearly an integer for $n = 1, 2, \dots, 7$ and that the closeness of the approximations decreases from about 10^{-12} at $n = 1$ to 10^{-2} at $n = 7$. Hence the observation made at (v) above will not apply from $n = 9$ onwards (remember

that only odd powers of n are relevant). Thus there is no reason to expect the large terms in the continued fraction for the root to persist beyond about the 200th term, i.e. about the point where the factor $1 + e^{-7\pi\sqrt{163}}$ has an effect. *This prediction is borne out.* We have computed the continued fraction to 875 terms and there are no large terms after the one shown in Table 1 at position 161.

Secondly, the last negative discriminant with class number 1 is -163 ; the penultimate is -67 and the one before that is -43 . The theory of modular functions shows that $e^{\pi\sqrt{67}}$ and $e^{\pi\sqrt{43}}$ will also be close to integers, and in fact:

$$\begin{aligned} e^{\pi\sqrt{67}} &= 147194952743.99999\ 86624\ 54224\dots, \\ e^{\pi\sqrt{43}} &= 884736743.99977\ 74660\ 34906\dots. \end{aligned}$$

The class invariants associated with these numbers also satisfy cubic equations. Is it possible that the continued fractions of the roots of these equations will also have large partial quotients for reasons similar to the above? The cubic equation associated with discriminant -67 is $x^3 - 2x^2 - 2x - 2 = 0$; expansion of the root showed one large partial quotient, 87431, at the 20th position. This is considerably larger than one would expect at random. The cubic associated with discriminant -43 is

$$x^3 - 2x^2 - 2 = 0;$$

again just one large partial quotient, 29,866, was found at the 17th position. A large number of other, random cubics were tested but none produced any unusually large partial quotients. It is a pity that -163 is the last of these interesting discriminants. Had there been another we might have seen some really astronomical partial quotients.

In cases where the class number is greater than one the term $-N$ of (9) is replaced by an algebraic number of degree greater than one. Thus, for example, if $d \equiv 3 \pmod{8}$ the algebraic number appearing in (9) is of degree $h(-d)$, and the value of $f(i\sqrt{d})$ is of degree $3h(-d)$. This is why in the three cases considered above ($d = 43, 67, 163$) we had to deal with a cubic equation. For an account of such matters see Watson (1936).

In view of these computational confirmations of our analysis, plus a good deal of other computational evidence on related aspects too lengthy to give here, we have reached the conclusion that Brillhart's cubic must be regarded as a quite un-typical cubic and consequently provides no evidence relating to Gauss' Law and cubics in general.

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