Experimental Methods in Number Theory and in Analysis

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Experimentation in Mathematics (1)

In any science, experimentation plays a major role, and mathematics (which certain people consider, in my opinion wrongly, not to be a science) is no exception. It is however true that certain branches of mathematics are more prone to experimentation than others. Putting aside applied mathematics, number theory is probably the mathematical field in which the experimental approach is most important.

Indeed, so-called "natural" sciences (physics, chemistry, biology, etc...) justly consider mathematics as a tool (even though certain parts of theoretical physics are essentially mathematics). Number theory can in fact also be considered as a "natural" science since its fundamental objects of study are natural numbers. And indeed, it uses almost completely the arsenal of the rest of mathematics as a tool.

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Experimentation in Mathematics (2)

Experimentation in mathematics is evidently quite similar to that of any other science, and can be summarized in the following way.

As a first step (which is not usually voluntary, but comes often by accident), we start from an experimental observation, if possible surprising, new, or curious, obtained for instance after a simple computation. This is the first step of experimental research in science: the most important and exciting moment for a scientist is not "Eureka!, I found the solution", but rather "Hum, something peculiar is happening".

As a second step, one tries to find other examples of the observation, and if possible, thanks to the accumulated experience, obtain a plausible conjecture, or at least the beginning of a theory which explains the observations.

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Experimentation in Mathematics (3)

As a third step, one tries to find still more examples or generalizations, to convince oneself and others that the theory is valid. Often, at this stage it is necessary to modify slightly the theory to be compatible with the new observations. Of course, we may also find that the conjecture is simply false and must be scrapped.

As a fourth and last step, which is unique to mathematics (and closely related subjects such as combinatorics, computer science, certain parts of theoretical physics, etc...), one tries finally to prove the conjecture. This is certainly the most important step, but it is often the most boring (although of course some proofs are even more beautiful than the experiments which led to them).

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Tools: Software

To experiment in mathematics, one needs appropriate software. Although one can use commercial tools such as `Maple` or `Mathematica`, the vast majority of experiments done in number theory are done using either the non-free university package `Magma`, or the free package `Sage`, or other free packages such as `Gap` and `Pari/GP` which are in fact included in `Sage`, and evidently I strongly recommend the use of these free packages.

In all of these software packages, it is necessary to have at one's disposal a number of efficient algorithms. The necessary basic algorithms are multiprecision algorithms, for integers and for real numbers (which are two rather different types of objects), as well as algorithms for handling standard objects such as polynomials (sparse and non-sparse), power series, vectors, matrices, and so on.

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Tools: Convergence Acceleration (1)

In addition, there exist a number of algorithms which I like to call magical, for the most part invented after 1980, which are remarkably powerful and useful, and which have the additional advantage of being simple to program. I will mention three of them, among my favorites.

(1). Algorithms for convergence acceleration of series: very frequently, even though a series $S = \sum_{n\geq 0} u_n$ converges, its convergence is very slow (typical example $\sum_{n\geq 1} 1/n^2$). There are several methods for accelerating the convergence of such series, and therefore to compute S to hundreds of decimals if we so desire. We will see below why on earth it is necessary to compute so many decimals (apart from the fun of it). One such method, probably the oldest but still extremely useful, is the Euler–Mac Laurin summation formula, discovered a few years after Taylor's formula.

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Tools: Convergence Acceleration (2)

A much more recent method to accelerate convergence uses Chebychev polynomials for accelerating alternating series $\sum_{n\geq 0}(-1)^n u_n$ with $u_n \geq 0$: it only needs 2 or 3 programming lines in a high level language! It is based on the following idea: one writes u_n as the nth moment of some function $w(t)$: $u_n = \int_0^1 t^n w(t)\,dt$, and then

$$S = \sum_{n\geq 0}(-1)^n u_n = \int_0^1 \frac{w(t)}{1+t}\,dt\ .$$

It follows that if $P(t)$ is any polynomial, we have

$$S = \frac{1}{P(-1)}\int_0^1 w(t)\frac{P(-1)-P(t)}{1+t}\,dt + \frac{1}{P(-1)}\int_0^1 w(t)\frac{P(t)}{1+t}\,dt\ .$$

Tools: Convergence Acceleration (3)

However $(P(-1)-P(t))/(1+t)$ is still a polynomial, so if we write

$$\frac{1}{P(-1)}\frac{P(-1)-P(t)}{1+t}=\sum_{n=0}^{N-1}c_nt^n$$

(where N is the degree of P), we have

$$S=\sum_{n=0}^{N-1}c_na_n+R,\quad \text{where}\quad R=\frac{1}{P(-1)}\int_0^1 w(t)\frac{P(t)}{1+t}\,dt\ ,$$

so that, assuming that $w(t)\geq 0$ on $[0,1]$, we have

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Tools: Convergence Acceleration (4)

Up to a constant factor, the degree N polynomial which minimizes this expression is the polynomial $T_N(1-2t)$, where T_N is the Chebychev polynomial defined by $T_N(\cos(x)) = \cos(Nx)$.

Assume for instance that we only want to use (or that we only know) the values of a_n for $n \leq N$, which should produce an error of the order of 6^{-N}. We use the following algorithm, which is indeed a three-line algorithm:

Set $d \leftarrow (3+\sqrt{8})^N$, $d \leftarrow (d+1/d)/2$, $b \leftarrow -1$, $c \leftarrow -d$, and $s \leftarrow 0$. Then for $k=0$ until $k=N-1$, repeat the following:

$c \leftarrow b-c$, $s \leftarrow s+c\cdot a_k$, $b \leftarrow (k+N)(k-N)b/((k+1/2)(k+1))$.

The result is s/d.

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Tools: Numerical Integration (1)

(2). Second example: algorithms for numerical computation of definite integrals $\int_a^b f(t)\,dt$. There exist very old methods for doing that (Trapezoid, Simpson's, Gauss's), or more recent (Richardson's), but it is only in the 1970's that a group of Japanese scientists (Mori, Takahashi) found a really revolutionary method, infinitely more efficient than all others: the doubly exponential method (it applies to a much more restricted class than previous methods, but that class includes all functions that you or me would like to integrate). It permits the computation of integrals to thousands of decimal digits if desired (once again see below for the reason), which is absolutely impossible with previous methods; it can just as easily be applied to improper integrals, such as functions with integrable algebraic singularities at endpoints, or integrals where a and/or b is infinite. It can even be extended to deal with indefinite integrals and multiple integrals, and of course easily to contour integrals. Once more, it is very easy to program in a few lines.

Tools: Numerical Integration (2)

The basic idea is very simple: assume that we want to compute $S = \int_{-1}^{1} f(x)\,dx$ (an affine change of variable transforms any integral on a compact interval to such an integral). We then do the magical change of variable $x = \phi(t)$, with

$$\phi(t) = \tanh(\sinh(t)), \quad \text{where} \quad S = \int_{-\infty}^{\infty} f(\phi(t))\phi'(t)\,dt\ .$$

The function $F(t) = f(\phi(t))\phi'(t)$ tends to 0 extremely fast (as $2/e^{e^t}$, hence doubly exponentially), and to compute its integral from $-\infty$ to $+\infty$, we simply use the Riemann sum formula $S \approx h\sum_{n=-N}^{N} F(nh)$, with h and N suitably chosen. Analysis of the method and experiment shows that for instance $h = 1/128$ and $N = 332$ are sufficient to obtain 100 decimal digits!!!).

Tools: Numerical Integration (3)

For improper integrals, we must simply change the magical function. For instance:

– For $\int_0^\infty f(x)\,dx$, where $f(x)$ does not tend to 0 exponentially fast when $x \to \infty$, we choose $x = \phi(t) = e^{\sinh(t)}$.

– For $\int_0^\infty f(x)\,dx$, where $f(x)$ tends to 0 exponentially fast when $x \to \infty$, as $e^{-g(x)}$ say, where g is increasing and tends to infinity with x (for instance $g(x) = x$), we choose $x = \phi(t) = g^{-1}(e^{t-e^{-t}})$.

– For $\int_0^\infty f(x)\,dx$, where $f(x)$ is oscillatory (for instance $f(x) = \sin(x)/x$), we must adapt the function ϕ. For instance, if $f(x) = g(x)\sin(x)$ with $g(x)$ not oscillatory, we can choose $x = \phi(t) = (\pi/h)t/\left(1 - e^{-\sinh(t)}\right)$. Note that this depends on h.

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Three remarks: (a). The relative ignorance of this method by specialists in numerical analysis comes in particular from the fact that it is mainly useful for the computation of integrals to tens of decimals, which is often useless in numerical analysis, but certainly not in number theory.

(b). Considering its importance and its simplicity, it should be taught in the first years of university, at least in parallel with the other methods. I am willing to admit that there is a pedagogical problem: it is not easy to justify its validity rigorously. Note also that one can show that doubly exponential is optimal: it would be of no use for instance to use triply exponential methods.

(c). The method works when the function to integrate is the restriction to the real line of a complex analytic function whose poles are away from the line. However the function may also have reasonable (algebraic) singularities.

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Tools: Numerical Integration (5)

One version of the algorithm on $[-1,1]$ is the following: given a C^∞ function on $[-1,1]$, with an error ε, and a small integer $r \geq 2$, we are going to compute $\int_{-1}^{1} f(x)\,dx$ with an error less than to ε.

– Initialize: $h \leftarrow 1/2^r$, $e_1 \leftarrow e^h$, $e_2 \leftarrow 1$, and $i \leftarrow 0$.

– Precomputations, to be done once and for all: $c \leftarrow e_2 + 1/e_2$, $s \leftarrow e_2 - c$, $e_3 \leftarrow 2/\left(e^{2s}+1\right)$, $x[i] = 1 - e_3$, $w[i] \leftarrow ce_3(1+x[i])$, $e_2 \leftarrow e_1 e_2$. If $e_3 > \varepsilon$, set $i \leftarrow i+1$ and start again the precomputations. Otherwise, set $w[0] \leftarrow w[0]/2$, $n \leftarrow i$, $S \leftarrow 0$, and $p \leftarrow 2^r$ (note: we will always have $n \leq 20 \cdot 2^r$).

– L: Set $p \leftarrow p/2$ and $i \leftarrow 0$.

– While $i \leq n$ do the following: if $(2p) \nmid i$ or if $p = 2^{r-1}$ set $S = S + w[i](f(-x[i]) + f(x[i]))$. Then set $i \leftarrow i + p$.

– If $p \geq 2$, go back to L, otherwise the result is $pS/2^r$.

Tools: The LLL Algorithm (1)

(3). One last magical algorithm that I would like to mention is the LLL algorithm, the acronym coming from the name of its discoverers Arjen Lenstra, Hendrik Lenstra, and Laszlo Lovasz. It is considered as one of the most important algorithms invented in the second half of the twentieth century. I will not explain it here, although it is not difficult and quite easy to implement.

This algorithm has numerous applications, also well outside the field of mathematics, but in the examples I will give, the main application is to find linear or algebraic relations between real or complex numbers. I give two examples.

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Tools: The LLL Algorithm (2)

(a). Thanks to doubly exponential numerical integration or to series summation, it is easy to compute that

$$J=\int_0^{\alpha}\frac{\log(1-t)}{t}\,dt=-0.75539561953174146938652002 8\cdots\ ,$$

with $\alpha=(\sqrt{5}-1)/2$, the inverse of the golden ratio. Now since I have a good intuition, I believe that J should be a linear combination with rational coefficients of π^2 and of $\log^2(\alpha)$. Thanks to LLL, in 10^{-4} seconds we find that, at least to 28 decimal digits, we indeed seem to have:

$$J=\log^2(\alpha)-\frac{\pi^2}{10}\ .$$

I emphasize that this relation has been found without searching naively for the coefficients: I repeat, it is magical.

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Tools (7): The LLL Algorithm (3)

(b). The computation of the value of a certain transcendental function that we will meet later gives

$$F = -191657.832862547207471353448\cdots$$

I believe that F should be the root of a second degree equation with integer coefficients.

I give this to LLL, which again in less than 10^{-4} seconds tells me that, at least to 28 decimals digits of accuracy, F is indeed the root of the second degree polynomial

$$x^2 + 191025x - 121287375 .$$

Once again, this has been found without doing a systematic search. There remains to prove the above two assertions, but that is another story.

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Two Historical Examples (1)

I am now going to give a series of examples coming from number theory and also from analysis (restricted to the computation of series and integrals) to illustrate what I have said up to now. Cheating slightly with historical facts, one of the first numerical conjectures in analysis has been the famous formula

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{1}{1^2} + \frac{1}{2^2} + \frac{1}{3^2} + \frac{1}{4^2} + \cdots = \frac{\pi^2}{6} \ .$$

Let us stop for a moment to look at this formula from an experimental point of view.

Two Historical Examples (2)

First of all, it is absolutely necessary to compute numerically the series on the left hand side, which converges very slowly: if we compute as written a thousand terms (think of the poor mathematicians of the 18th century!), we only obtain 3 correct decimals. Luckily, geniuses such as Euler, Bernoulli, and others already knew methods for accelerating convergence. In fact, the Euler–Mac Laurin summation formula was invented essentially for this precise purpose, and it is only after the invention of this summation formula that any conjecture could be made on the value of the sum.

After the computation of the sum $1.644934066848\cdots$, it is of course necessary to guess that it is equal to $\pi^2/6$, which is not too difficult when one has some experience and/or one is a genius like Euler (it is much more difficult in the second example). There remains to prove the conjecture, and this harder. One way is to continue the experimental work: one finds that numerically one seems to have $\sum_{n\geq 1} 1/n^4 = \pi^4/90$, $\sum_{n\geq 1} 1/n^6 = \pi^6/945$, etc...

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The proof of these formulas is more difficult: although historically it did not happen in this way, it is in fact not too difficult to show that if we set $P = \sqrt{6\sum_{n\ge1} 1/n^2}$ (which should therefore be equal to π), then by definition $\sum_{n\ge1} 1/n^2 = P^2/6$, but also $\sum_{n\ge1} 1/n^4 = P^4/90$, $\sum_{n\ge1} 1/n^6 = P^6/945$, etc... The difficulty is in showing that $P = \pi$. This is a well-known undergraduate exercise: one can either first prove the elementary trigonometric identity

$$\sum_{1\le k\le n-1} \mathrm{cotan}^2(k\pi/2n) = \frac{(n-1)(2n-1)}{3}\ ,$$

from which the result follows by using the elementary estimate $\mathrm{cotan}^2(x) < 1/x^2 < 1 + \mathrm{cotan}^2(x)$ for $|x| < \pi/2$, or more naturally by the theory of Fourier series.

Two Historical Examples (4)

As a second example, I would like to mention the discovery by Gauss of the link between the arithmetic-geometric mean (AGM) and the lemniscatic integral (generalized later to all elliptic integrals), which illustrates the incredible intuition of Gauss.

The AGM $\text{agm}(a, b)$ of two positive real numbers a et b is defined as the common limit of the two sequences defined by $a_0 = a$, $b_0 = b$, and $a_{n+1} = (a_n + b_n)/2$, $b_{n+1} = \sqrt{a_n b_n}$. It is very easy to show that the two sequences converge to the same limit, and very rapidly. At the age of 18, Gauss "observes" experimentally that to more than 10 decimal digits we have

$$\frac{1}{\text{agm}(1, \sqrt{2})} = \frac{2}{\pi} \int_0^1 \frac{dt}{\sqrt{1 - t^4}} .$$

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As mentioned, the numerical computation of the AGM on the left is extremely fast. The integral on the right is known as the lemniscatic integral, and its value was given in the books on integrals at Gauss's disposal. What is really amazing is that he had the intuition to compute specifically the AGM of 1 and of $\sqrt{2}$, then to compute its inverse, and finally to multiply the integral by $2/\pi$ (and also he had no a priori reason to think that there was any link between the left hand side and the integral).

As Gauss himself said, this discovery (which he indeed proved not long after, it is not difficult once you get a hint) will open an entirely new field of mathematics, and indeed it was the beginning of the vast theory of elliptic functions developed in the 19th century by Gauss, Weierstrass, Jacobi, and others.

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Numerology or not (1) ?

Any computer algebra system will tell you that

$$e^{\pi\sqrt{163}} = 262537412640768743.99999999999925007259\cdots$$

Is this a numerical coincidence ? Even though you have probably seen this example before, I want to convince you in two different ways that it is not a coincidence.

First of all, we can try to replace 163 by other integers, or even by other rational numbers. Indeed, we find for instance that

$$e^{\pi\sqrt{67}} = 147197952743.9999986624542\cdots$$

$$e^{\pi\sqrt{43}} = 884736743.9997774660349\cdots$$

Less spectacular of course, but not too bad.

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Numerology or not (2) ?

We can make the above examples much more striking by noticing that the numbers all end with $743.999\cdots$. In addition, if we compute the cube root after subtracting 744, it remains extremely close to an integer!!! Thus:

$$(e^{\pi\sqrt{163}} - 744)^{1/3} = 640319.99999999999999999999999939031\cdots$$
$$(e^{\pi\sqrt{67}} - 744)^{1/3} = 5279.9999999999999840073\cdots$$
$$(e^{\pi\sqrt{43}} - 744)^{1/3} = 959.99999999919511\cdots$$

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Numerology or not (3) ?

Convinced that we are now confronted with an interesting phenomenon, the second step consists in trying to understand the phenomenon more closely, by finding more precise identities or analogous examples.

In the present case, let us continue experimenting with the same data. We are going to set $q = e^{-\pi\sqrt{163}} = 3.8089 \cdots 10^{-18}$, and try to go further in the approximation. We have seen that $1/q = e^{\pi\sqrt{163}}$ is very close to the integer $N = 262537412640768744$. More precisely, we compute that $N - 1/q = 7.499274 \cdots 10^{-13}$. Until now, nothing new.

However q also is very small! With a sudden inspiration, we divide the error $N - 1/q$ by q, and we find:

$$(N - 1/q)/q = 196883.999999999918130 \cdots$$

Curiouser and curiouser!. It follows that N is very close to $1/q + 196884q$.

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Numerology or not (4) ?

There is of course no reason to stop there. In the same way, we compute that the new error divided by q^2 is:

$$(N - (1/q + 196884q))/q^2 = -21493759.999999996707\cdots ,$$

again very close to an integer, so N is very close to $1/q + 196884q - 21493760q^2$.

Continuing in this way, we find that apparently $N = S(q)$ with

$$\begin{aligned} S(q) = \frac{1}{q} &+ 196884q - 21493760q^2 + 864299970q^3 \\ &- 20245856256q^4 + 333202640600q^5 \\ &- 4252023300096q^6 + 44656994071935q^7 \\ &- 401490886656000q^8 + 3176440229784420q^9 + \cdots \end{aligned}$$

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Numerology or not (5) ?

This is absolutely remarkable. However there still remains one thing to check before stopping this specific experimentation: is the series in q that we just obtained linked in some way to the number 163, or is it universal ?

Thus, to check this, let us replace 163 by 67. We can either do the same thing to check whether the coefficients are the same (this is indeed the case), or directly set $q = e^{-\pi\sqrt{67}}$ in the above series, and see whether we get an integer. Recall that $e^{\pi\sqrt{67}} = 147197952743.99999866\cdots$, which is not too bad but not so amazing.

Indeed, we find that

$$S\left(e^{-\pi\sqrt{67}}\right) = 147197952744 + 4.72\cdots 10^{-96}$$
$$S\left(e^{-\pi\sqrt{43}}\right) = 8847836744 + 7.67\cdots 10^{-74},$$

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Numerology or not (6) ?

Is this really always true ? In fact, I cheated and forgot on purpose to mention that it also works for 58: we have

$$e^{\pi\sqrt{58}} = 24591257751.99999982221\cdots$$

Here, we check that the series $S(q)$ does not work. Exactly in the same way, we find instead that the series which does work for 58 is the series

$$T(q) = 1/q + 4372q + 96256q^2 + 1240002q^3 + 10698752q^4 + 74428120q^5 + 431529984q^6 + \cdots$$

If we write a small program, one checks that $S(e^{-\pi\sqrt{D}})$ is Very Close to an Integer (much closer than $e^{\pi\sqrt{D}}$ itself), which we abbreviate to VCI for $D = 3, 7, 11, 19, 27, 43, 67, 163$, that $S(-e^{-\pi\sqrt{D}})$ is VCI for $D = 4, 8, 12, 16, 28,$

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Numerology or not (7) ?

that $T(e^{-\pi\sqrt{D}})$ is VCI for $D = 4, 6, 10, 18, 22, 58$, and that $T(-e^{-\pi\sqrt{D}})$ is VCI for $D = 5, 7, 9, 13, 25, 37$.

The experimental part is far from being finished: if we set

$$U(q) = 1/q + 79q - 352q^2 + 1431q^3 - 4160q^4 + 13015q^5 - 31968q^6 + 81162q^7 + \cdots ,$$

then $U(e^{-\pi\sqrt{D}})$ is VCI for $D = 5/3, 7/3, 11/3, 19/3, 31/3, 59/3$, $U(-e^{-\pi\sqrt{D}})$ is VCI for $D = 2, 4/3, 10/3, 14/3, 26/3, 34/3$, and if

$$V(q) = 1/q + 783q - 8672q^2 + 65367q^3 - 371520q^4 + \cdots ,$$

then $V(e^{-\pi\sqrt{D}})$ is VCI for $D = 17/3, 25/3, 41/3, 49/3, 89/3$, and $V(-e^{-\pi\sqrt{D}})$ is VCI for $D = 16/3, 20/3$.

For an example with larger denominators, if

$$W(q) = 1/q + 9q^2 - 6q^3 + 4q^4 + 46q^5 + 79q^6 + \cdots ,$$

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Numerology or not (8) ?

Although there still remains experiments to be done on this subject, I will stop here. Of course we must now understand what these series $S(q)$, $T(q)$, etc... are, and what are these rational numbers $D = 3, 7, 11, 19, 27, 43, 67, 163$, etc...

The series $S(q)$,... are called modular functions, and more precisely in our case they are called Hauptmoduln: for instance, if we set

$$\eta(q) = q^{1/24}\prod_{n\geq 1}(1-q^n) \quad \text{and} \quad E_4(q) = 1 + 240\sum_{n\geq 1} n^3 \frac{q^n}{1-q^n}$$

(of course you do not need to have any knowledge of modular forms to understand these definitions, but you do need this knowledge to understand where they originate from), we have

$$S(q)-744 = \frac{E_4(-q)^3}{\eta(-q)^{24}} \quad \text{and} \quad T(q)-24 = \left(\frac{\eta(q)}{\eta(q^2)}\right)^{24} + 4096\left(\frac{\eta(q^2)}{\eta(q)}\right)^{24}$$

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Numerology or not (9) ?

The phenomenon that we have observed (the fact that the values of the modular functions are integral (more precisely VCI) for certain values of D) is at the heart of the theory of complex multiplication. In fact, we can observe a phenomenon which is closely connected to this: For the values of D given above which are not divisible by 3 ($D = 7, 11, 19, 43, 67, 163$), the polynomial $x^2 + x + (D+1)/4$ takes only prime values for $0 \leq x < (D-3)/4$, the most spectacular being Euler's polynomial $x^2 + x + 41$ which gives prime numbers for all x such that $0 \leq x < 40$.

Other non numerological phenomena (1)

It is of course easy to give many examples of apparent numerological facts which come in fact from very serious mathematical theories. I give two such examples. First, recall that

$$4\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{2n-1}=4\left(1-\frac{1}{3}+\frac{1}{5}-\frac{1}{7}+\cdots\right)=\pi\ .$$

The convergence of this series is slow (in fact the same speed as $\sum 1/n^2$): for instance one needs 1 million terms to have 6 decimals. It is in fact easy to modify the Chebychev-based acceleration method explained above to compute this series, but it is not my purpose here. Instead, let us compute the sum S of the first 500000 terms. We find that $S=3.1415906\cdots$, while $\pi=3.1415926\cdots$, whence an error of $2\cdot 10^{-6}$, which is exactly what is expected.

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Nothing surprising up to now. Nonetheless, without computing any more terms, let us compute S to more decimals. We find that

$$S = 3.14159065358979324\text{0}, \quad \text{while}$$
$$\pi = 3.14159265358979323\text{8} .$$

Thus, even though the 6th decimal is wrong, the next 9 are correct! And this goes on! We have

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and we can continue this game a long time. This phenomenon is a simple consequence of the Euler–Mac Laurin summation formula that we already mentioned.

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Other non numerological phenomena (3)

For another example, I give the following very pretty false identity:

$$\sum_{n=1}^{\infty} e^{-(n/10)^2} = 5\sqrt{\pi} - \frac{1}{2} \, .$$

If we want to check this on a computer, we indeed find that both sides are equal to $8.3622692545275\cdots$, even if we do the computation to 100 decimals. Nonetheless, the identity is false, but it is necessary to work to more than 430 decimals to notice it, since the difference between the right and left hand side is of the order of 10^{-427}. Once again, this type of numerology has a mathematical explanation: here it is the functional equation of the theta function.

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A Difficult Integral (1)

During the CNTA meeting in Montreal in 2002, H. Muzzafar announced that he knew how to compute explicitly integrals of the type

$$J(a) = \int_0^1 \frac{\log(1+t^a)}{1+t}\, dt\ ,$$

where a is a real quadratic unit, in other words a root of an equation of the type $x^2 - tx \pm 1 = 0$, and he challenged the audience to prove the identities that he obtained in an “elementary” way. Indeed, since then I have not succeeded in doing so, and I have not even been able to reproduce the author’s proof (although I know where to look in the old German literature to find suitable pointers). Using the tools of numerical integration and the LLL algorithm (this is where it is essential to compute the series and the integrals to hundreds of decimal digits), I have noticed experimentally that the following identities are true to several hundred digits of accuracy (which of course does not prove anything, see the preceding example):

A Difficult Integral (2)

$$J(1+\sqrt{2}) = \frac{\log^2(2)}{2} + \frac{\log(2)\log(1+\sqrt{2})}{2} - \frac{\pi^2}{24},$$

$$J(3+2\sqrt{2}) = \frac{\log^2(2)}{2} + \frac{3\log(2)\log(1+\sqrt{2})}{2} + \frac{3\pi^2}{8} - \frac{\pi^2(3+2\sqrt{2})}{12},$$

$$J(2+\sqrt{3}) = \frac{\log^2(2)}{2} + \frac{\log(2)\log(2+\sqrt{3})}{2} + \frac{\pi^2}{4} - \frac{\pi^2(2+\sqrt{3})}{12},$$

$$J(2+\sqrt{5}) = \frac{\log^2(2)}{2} + \frac{2\log(2)\log(2+\sqrt{5})}{3} - \frac{\pi^2}{12},$$

$$J(4+\sqrt{17}) = \frac{\log^2(2)}{2} + \log(2)\log(4+\sqrt{17}) - \frac{\pi^2}{6},$$

$$J(4+\sqrt{15}) = \log(2)\log(\sqrt{3}+\sqrt{5}) + \log(2+\sqrt{3})\log\left(\frac{1+\sqrt{5}}{2}\right) + \frac{\pi^2}{2} - \frac{\pi^2(4+\sqrt{15})}{12}.$$

Exercise: compute explicitly $J(6+\sqrt{35})$ and $J(12+\sqrt{143})$, and generalize the above evaluations to $\int_0^1 \operatorname{atan}(t^a)/(1+t^2)\,dt$.

A Difficult Integral (2)

$$J(1+\sqrt{2}) = \frac{\log^2(2)}{2} + \frac{\log(2)\log(1+\sqrt{2})}{2} - \frac{\pi^2}{24},$$

$$J(3+2\sqrt{2}) = \frac{\log^2(2)}{2} + \frac{3\log(2)\log(1+\sqrt{2})}{2} + \frac{3\pi^2}{8} - \frac{\pi^2(3+2\sqrt{2})}{12},$$

$$J(2+\sqrt{3}) = \frac{\log^2(2)}{2} + \frac{\log(2)\log(2+\sqrt{3})}{2} + \frac{\pi^2}{4} - \frac{\pi^2(2+\sqrt{3})}{12},$$

$$J(2+\sqrt{5}) = \frac{\log^2(2)}{2} + \frac{2\log(2)\log(2+\sqrt{5})}{3} - \frac{\pi^2}{12},$$

$$J(4+\sqrt{17}) = \frac{\log^2(2)}{2} + \log(2)\log(4+\sqrt{17}) - \frac{\pi^2}{6},$$

$$J(4+\sqrt{15}) = \log(2)\log(\sqrt{3}+\sqrt{5}) + \log(2+\sqrt{3})\log\left(\frac{1+\sqrt{5}}{2}\right) + \frac{\pi^2}{2} - \frac{\pi^2(4+\sqrt{15})}{12}.$$

Exercise: compute explicitly $J(6+\sqrt{35})$ and $J(12+\sqrt{143})$, and generalize the above evaluations to $\int_0^1 \operatorname{atan}(t^a)/(1+t^2)\,dt$.

The Birch and Swinnerton-Dyer Conjecture (1)

Although it involves slightly more advanced notions, in my opinion the Birch and Swinnerton-Dyer (BSD) conjecture is one of the most elegant and important problems in the whole of mathematics (notwithstanding the fact that it is one of the 1 million $ Clay problems). It is a typical example of modern experimental mathematics.

In the 1960's, two British mathematicians, Bryan Birch and Peter Swinnerton-Dyer (now Sir Peter), computed numerically an analytic quantity called "the value at 1 of the L-function of elliptic curves". No need to define precisely this here, but they observed, and of course this is part of their experimental genius, that this value seemed to vanish if and only if the elliptic curve had an infinity of points with rational coordinates.

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The Birch and Swinnerton-Dyer Conjecture (2)

Soon after, they generalized this observation, which I repeat was purely experimental, by giving a precise relationship between the leading coefficient of the Taylor expansion of the L-function at 1 and purely algebraic and arithmetic invariants of the elliptic curve. I emphasize that even in its initial formulation the BSD conjecture remains unproved.

Many theorems, for the most part deep and difficult, have been proved on this conjecture, by some of the best number theorists in the world (Coates–Wiles, Kolyvagin, Gross–Zagier, Rubin, Nekovar,...). Nonetheless one can say that the conjecture is far from being solved. Although I do not want to give the precise definitions, I will give a general idea based on some examples, either related to Diophantine problems, or purely numerical.

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Although I do not want to give the precise definitions, I will give a general idea based on some examples, either related to Diophantine problems, or purely numerical.

The Birch and Swinnerton-Dyer Conjecture (3)

As a first example, consider the problem of representing an integer or a rational number c as a sum of two cubes of rational numbers, in other words the Diophantine equation $c = a^3 + b^3$, with a and b in $\mathbb{Q}$. Clearing denominators, this is equivalent to the solubility in integers of the equation $x^3 + y^3 = cz^3$ with $z \neq 0$. For instance the number 15 is representable since

$$15 = (397/294)^3 + (683/294)^3 \ ,$$

and it is the simplest representation. On the contrary, one can show that the number 14 is not representable.

A consequence of the BSD conjecture, which is also far from being proved, is that any squarefree integer (not divisible by a square other than 1) and congruent to 4, 6, 7, or 8 modulo 9 is indeed a sum of two cubes of rational numbers. Note that BSD does not give us any such representation, and that the converse is false: for instance $91 = 3^3 + 4^3$ although $91 \equiv 1 \pmod 9$.

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As a second example, I mention the congruent number problem. It is I believe the last problem coming from the ancients Greeks that is still not completely solved! Let me give some definitions: an integer S is called congruent if it is equal to the area of a Pythagorean triangle, in other words a right-angled triangle with all sides rational, such as the well-known triangle $(3, 4, 5)$, with area 6, which shows that 6 is a congruent number. The problem is to give a simple characterization of congruent numbers. The BSD conjecture gives a complete answer to this problem, in two different ways, but I will mention only one of them (the least elegant, but closest to what I want to show).

One can of course always reduce to the case where S is squarefree. In that case, analogously to the problem of sums of two cubes, BSD predicts that if S is congruent to 5, 6 or 7 modulo 8 then S is indeed congruent (as usual without giving any indication on the corresponding Pythagorean triangle).

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The Birch and Swinnerton-Dyer Conjecture (5)

For S congruent to 1, 2, or 3 modulo 8, the condition is more difficult to explain, so please forgive me if I now give technical details. Let us define an arithmetic function $a(n)$ in the following way. Set $a(1) = 1$ and otherwise:

(1). For $n = p$ prime, set $a(p) = 0$ if $p \mid S$, or if $p = 2$, or if $p \equiv 3 \pmod 4$. Otherwise we have $p \equiv 1 \pmod 4$, so by a well-known theorem due to Fermat there exist a and b such that $p = a^2 + b^2$, and without loss of generality we may assume that $a \equiv -1 \pmod 4$. We set $a(p) = -2a$ if $2S$ is a square modulo p, and $a(p) = 2a$ otherwise.

(2). If $k \geq 2$ and p is prime, we define $a(p^k)$ by the recursion

$$a(p^k) = a(p)a(p^{k-1}) - \chi(p)pa(p^{k-2}) \ ,$$

where $\chi(p) = 1$ except when $p \mid 2S$, in which case $\chi(p) = 0$.

(3). Finally, for an arbitrary n we set

$$a(n) = \prod_{i=1}^{g} a(p_i^{k_i}), \quad \text{where} \quad n = \prod_{i=1}^{g} p_i^{k_i} \ .$$

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Assuming the BSD conjecture, the result is then as follows: if S is a squarefree integer congruent to 1, 2, or 3 modulo 8, then S is a congruent number if and only if

$$\sum_{n=1}^{\infty} \frac{a(n)}{n} e^{-\pi n/(2S\sqrt{\delta})} = 0 ,$$

where $\delta = 1$ if S is even, and $\delta = 2$ if S is odd.

This admittedly very complicated statement is in fact a reformulation of BSD in the context of congruent numbers; however I emphasize that the series is very easy to compute since the convergence is fast. On the other hand, proving that the sum is exactly equal to 0 cannot be done numerically: indeed, if a certain mathematical quantity is different from 0, this can be proved numerically on a computer by taking sufficient accuracy, but if some other mathematical quantity is equal to 0 this cannot be proved on a computer. In the present case, it can be proved mathematically.

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The Birch and Swinnerton-Dyer Conjecture (7)

Let me give two examples of this: if $S = 210$ then one can prove that the above sum is exactly equal to 0. For experts: in this case, the elliptic curve has algebraic rank equal to 2 and sign of the functional equation $+1$. If the above sum, equal up to a nonzero factor to the value at 1 of the L-function, was not equal to 0, then by the known results on BSD (here the Coates–Wiles theorem) the algebraic rank would be equal to 0, a contradiction.

The same phenomenon is true for $S = 29274$: the above sum is indeed exactly equal to 0. However in this case the BSD conjecture says more. (For experts: this is a curve of algebraic rank 4, and we will compute the second derivative of the L-function at 1.)

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The Birch and Swinnerton-Dyer Conjecture (8)

For any $x > 0$ define a function f by the formula

$$f(x) = \int_1^\infty e^{-xt} \log(t)^2 \, dt \; ,$$

and let T be the series

$$T = \sum_{n=1}^{\infty} a(n) f\left(\frac{2\pi n}{4 \cdot 29274}\right) \; ,$$

which also converges exponentially fast since $f(x) \sim 2e^{-x}/x^3$.
An easy numerical computation shows that to thousands of decimal digits T is close to 0. However this is a conjecture: even though it is a special case of BSD, it is almost certainly as difficult to prove as the general case, which is of the same type.

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A Scoop (1)

To finish, I will show you a piece of numerical evidence which is still unexplained.

Recall that a Dirichlet character χ modulo N is an arithmetic function such that $\chi(xy) = \chi(x)\chi(y)$, $\chi(x+N) = \chi(x)$, and $\chi(x) = 0$ if and only if $\gcd(x, N) > 1$. It is primitive if it is not the restriction of a character coming from some nontrivial divisor of N. If $\chi(-1) = 1$ (χ even), we associate the theta function

$$\theta(\chi, t) = \sum_{n \geq 1} \chi(n) e^{-\pi n^2 t/N} \ .$$

(if $\chi(-1) = -1$, replace $\chi(n)$ by $n\chi(n)$).

By the Poisson summation formula we have

$$\theta(\chi, 1/t) = \varepsilon(\chi) t^{1/2} \theta(\overline{\chi}, t) \ ,$$

where $|\varepsilon(\chi)| = 1$ is the so-called root number, easily expressible in terms of Gauss sums.

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This implies the well-known functional equation of the L-function:

$$\Lambda(1-s,\chi)=\varepsilon(\chi)\Lambda(s,\overline{\chi}) \quad \text{where} \quad \Lambda(s,\chi)=\pi^{-s/2}\Gamma(s/2)L(s,\chi)\;.$$

Efficient method to compute $\varepsilon(\chi)$:

$$\varepsilon(\chi)=\frac{\theta(\chi,1)}{\theta(\overline{\chi},1)}\;,$$

if denominator nonzero (otherwise can choose $t\neq 1$ close to 1).

Question: can we have

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Conjectural answer by Louboutin: never.

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However conjecture probably false: nearly 5 million primitive characters modulo $N \leq 5000$ exist, apparently TWO (closely related) counterexamples (and their conjugates). Specifically:

$$(\mathbb{Z}/300\mathbb{Z})^* = (\mathbb{Z}/20\mathbb{Z})[277] \oplus (\mathbb{Z}/2\mathbb{Z})[151] \oplus (\mathbb{Z}/2\mathbb{Z})[101] \ .$$

Define

$$\chi(277) = e^{4i\pi/5} \quad \chi(151) = \chi(101) = -1 \ ,$$

so χ is an even primitive character modulo 300 of order 10.

Then apparently

$$\theta(\chi, 1) = \sum_{n\geq 1} \chi(n) e^{-\pi n^2/300} = 0 \ ,$$

at least to 10000 decimals.

Questions:

¿ How does one prove this ?

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