9

Irregular continued fractions

We finish our expedition with a look at irregular continued fractions and pass by some classical gems en route.

9.1 General theory

There exist many generalisations of classical continued fractions. One of the most natural generalisations, which admits many applications not only in number theory but also in analysis, is the following *irregular continued fraction*:

$$a_0 + \cfrac{b_1}{a_1 + \cfrac{b_2}{a_2 + \cfrac{b_3}{a_3 + \ddots + a_{n-1} + \cfrac{b_n}{a_n}}}},$$

which is written as

$$a_0 + \frac{b_1|}{|a_1} + \frac{b_2|}{|a_2} + \frac{b_3|}{|a_3} + \cdots + \frac{b_n|}{|a_n}.$$

For the regular continued fractions considered earlier, we have $b_n = 1$ for all n.

An *infinite irregular continued fraction* can then be written as

$$a_0 + \frac{b_1|}{|a_1} + \frac{b_2|}{|a_2} + \frac{b_3|}{|a_3} + \cdots + \frac{b_n|}{|a_n} + \cdots \tag{9.1}$$

and is formalised as follows. For two given sequences of numbers or indeterminates $(a_n)_{n=0}^{\infty}$ and $(b_n)_{n=1}^{\infty}$, we define rational functions $S_n(x)$ by the rule

$$S_0(x) = a_0 + x, \qquad S_n(x) = S_{n-1}\left(\frac{b_n}{a_n + x}\right), \quad n = 1, 2, 3, \ldots$$

By induction on $n = 1, 2, \dots$ it is not hard to show that

$$S_n(x) = a_0 + \frac{b_1|}{|a_1} + \frac{b_2|}{|a_2} + \frac{b_3|}{|a_3} + \cdots + \frac{b_n|}{|a_n + x}.$$

Therefore, $r_0 = S_0(0) = a_0$ and

$$r_n = S_n(0) = a_0 + \frac{b_1|}{|a_1} + \frac{b_2|}{|a_2} + \frac{b_3|}{|a_3} + \cdots + \frac{b_n|}{|a_n}, \qquad n = 1, 2, 3, \dots$$

If we assign numerical values to the sequences $(a_n)_{n=0}^{\infty}$ and $(b_n)_{n=1}^{\infty}$ (assuming that $b_n \neq 0$ for $n \in \mathbb{N}$) then we can consider the limit

$$\alpha = \lim_{n \to \infty} r_n.$$

If this limit exists α is said to be the *value* of the irregular continued fraction (9.1); the numbers r_n, where $n = 0, 1, 2, \dots$, are called the nth *convergents*.

As in the case of regular continued fractions, to every continued fraction (9.1) we assign the sequences of numerators $(p_n)_{n=-1}^{\infty}$ and denominators $(q_n)_{n=-1}^{\infty}$ of the convergents. They are determined by the linear recurrence equations

$$\begin{aligned} &p_{-1} = 1, \quad p_0 = a_0, \qquad p_n = a_n p_{n-1} + b_n p_{n-2}, \quad n = 1, 2, \dots, \\ &q_{-1} = 0, \quad q_0 = 1, \qquad q_n = a_n q_{n-1} + b_n q_{n-2}, \quad n = 1, 2, \dots \end{aligned} \tag{9.2}$$

(When $b_n \equiv 1$ we have our familiar regular continued fraction recursions.)

The fact that these sequences indeed provide the numerators and denominators of the corresponding convergents is proved in the following statement.

Theorem 9.1 *If p_n and q_n are the sequences generated by* (9.2) *for a given continued fraction* (9.1) *and $S_n(x)$ is the above sequence of rational transformations then*

$$S_n(x) = \frac{p_n + p_{n-1}x}{q_n + q_{n-1}x}, \quad p_n q_{n-1} - p_{n-1} q_n \neq 0, \qquad n = 0, 1, 2, \dots$$

In particular,

$$r_n = S_n(0) = \frac{p_n}{q_n}, \qquad n = 0, 1, 2, \dots$$

Exercise 9.2 Prove Theorem 9.1 by induction on $n = 0, 1, 2, \dots$

Once again, a 2×2 matrix approach is useful. From the recurrence relations in (9.2), we see that

$$\begin{pmatrix} a_0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a_1 & 1 \\ b_1 & 0 \end{pmatrix} \cdots \begin{pmatrix} a_n & 1 \\ b_n & 0 \end{pmatrix} = \begin{pmatrix} p_n & p_{n-1} \\ q_n & q_{n-1} \end{pmatrix}.$$

By taking the determinant of both sides, we obtain immediately

Corollary 9.3 *We have*

$$p_nq_{n-1} - p_{n-1}q_n = (-1)^{n-1}\prod_{k=1}^{n} b_k \qquad \text{for } n = 0, 1, 2, \ldots$$

Summarising, the sequence of convergents of a continued fraction (9.1) is uniquely determined by the sequences $(p_n)_{n=-1}^{\infty}$ and $(q_n)_{n=-1}^{\infty}$, which, in turn, are constructed by means of the recurrence relations (9.2). As the following theorem shows, the converse holds as well: the sequences (9.2) define the continued fraction (9.1) in a unique way.

Theorem 9.4 *Let $(p_n)_{n=-1}^{\infty}$ and $(q_n)_{n=-1}^{\infty}$ be two sequences of numbers such that $q_{-1} = 0$, $p_{-1} = q_0 = 1$ and $p_nq_{n-1} - p_{n-1}q_n \neq 0$ for $n = 0, 1, 2, \ldots$ Then there exists a unique continued fraction* (9.1) *whose nth numerator is b_n and nth denominator is a_n, for each $n \geq 0$. More precisely,*

$$a_0 = p_0, \quad a_1 = q_1, \quad b_1 = p_1 - p_0q_1,$$
$$\left.\begin{aligned} a_n &= \frac{p_nq_{n-2} - p_{n-2}q_n}{p_{n-1}q_{n-2} - p_{n-2}q_{n-1}}, \\ b_n &= \frac{p_{n-1}q_n - p_nq_{n-1}}{p_{n-1}q_{n-2} - p_{n-2}q_{n-1}}, \end{aligned}\right\} \quad n = 2, 3, \ldots$$

Proof Again, the proof is by induction on $n = 0, 1, 2, \ldots$ □

Theorem 9.1 provides us with a simple algorithm for computing the value of an irregular continued fraction. Namely,

$$\begin{aligned} r_n = \frac{p_n}{q_n} &= p_0 + \sum_{l=1}^{n}\left(\frac{p_l}{q_l} - \frac{p_{l-1}}{q_{l-1}}\right) \\ &= a_0 + \sum_{l=1}^{n} \frac{(-1)^{l-1}\prod_{k=1}^{l} b_k}{q_lq_{l-1}}, \qquad n = 0, 1, 2, \ldots, \end{aligned}$$

implying that

$$a_0 + \frac{b_1|}{|a_1} + \frac{b_2|}{|a_2} + \frac{b_3|}{|a_3} + \cdots + \frac{b_n|}{|a_n} + \cdots = a_0 + \sum_{l=1}^{\infty} \frac{(-1)^{l-1}\prod_{k=1}^{l} b_k}{q_lq_{l-1}}.$$

Therefore, the convergence problem for continued fractions of the form (9.1) can be reduced to a convergence problem for the corresponding series.

Two (irregular) continued fractions

$$a_0 + \frac{b_1|}{|a_1} + \frac{b_2|}{|a_2} + \frac{b_3|}{|a_3} + \cdots + \frac{b_n|}{|a_n} + \cdots \quad \text{and} \quad a_0' + \frac{b_1'|}{|a_1'} + \frac{b_2'|}{|a_2'} + \frac{b_3'|}{|a_3'} + \cdots + \frac{b_n'|}{|a_n'} + \cdots \tag{9.3}$$

with corresponding sequences of convergents $(r_n)_{n=0}^{\infty}$ and $(r'_n)_{n=0}^{\infty}$, respectively, are said to be *equivalent* if

$$r_n = r'_n \qquad \text{for all } n = 0, 1, 2, \dots$$

Theorem 9.5 *Two continued fractions* (9.3) *are equivalent iff there exists a sequence of nonzero numbers* $(c_n)_{n=0}^{\infty}$ *with* $c_0 = 1$ *such that*

$$a'_n = c_n a_n, \quad n = 0, 1, 2, \dots, \qquad b'_n = c_n c_{n-1} b_n, \quad n = 1, 2, \dots \tag{9.4}$$

Proof First, assume that relations (9.4) hold. Then it can be easily shown by induction on $n = 0, 1, 2, \dots$, with the help of the recurrence relations (9.2), that

$$p'_n = p_n \prod_{l=0}^{n} c_l, \qquad q'_n = q_n \prod_{l=0}^{n} c_l, \tag{9.5}$$

implying that $r'_n = p'_n/q'_n = p_n/q_n = r_n$. Second, if $r'_n = r_n$ for all $n = 0, 1, 2, \dots$ then take $c_0 = 1$ and define recursively $c_n = p'_n/(p_n \prod_{l=0}^{n-1} c_l)$. Now we arrive at the relations in (9.5), which imply (9.4) in accordance with the formulae of Theorem 9.4. □

Finally, we stress that the value of an infinite *irregular* continued fraction is not necessarily an irrational number even when the a_k and b_k are required to be positive integers. An example is given in the following exercise.

EXERCISE 9.6 Compute the value of the continued fraction

$$1 + \frac{2|}{|1} + \frac{2|}{|1} + \frac{2|}{|1} + \cdots + \frac{2|}{|1} + \cdots .$$

9.2 Euler continued fraction

Finite identities such as

$$a_0 + a_1 + a_1a_2 + a_1a_2a_3 + a_1a_2a_3a_4 = a_0 + \frac{a_1|}{|1} + \frac{a_2|}{|1 + a_2} + \frac{a_3|}{|1 + a_3} + \frac{a_4|}{|1 + a_4}$$

are easily verified symbolically. The general form

$$\begin{aligned} &a_0 + a_1 + a_1a_2 + a_1a_2a_3 + \cdots + a_1a_2a_3 \cdots a_N \\ &\quad = a_0 + \frac{a_1|}{|1} + \frac{a_2|}{|1 + a_2} + \frac{a_3|}{|1 + a_3} + \cdots + \frac{a_N|}{|1 + a_N} \end{aligned} \tag{9.6}$$

can then be obtained by substituting $a_N + a_N a_{N+1}$ for a_N and checking that the form of the right-hand side is preserved.

Equation (9.6) allows many series to be re-expressed as irregular continued fractions. For example, with $a_0 = 0$, $a_1 = z$, $a_2 = -z^2/3$, $a_3 = -3z^2/5, \ldots$, we find that

$$\arctan z = z - \frac{z^3}{3} + \frac{z^5}{5} - \frac{z^7}{7} + \frac{z^9}{9} - \cdots \tag{9.7}$$

with $|z| \le 1$, can be expressed as an irregular continued fraction due to Euler:

$$\arctan z = \frac{z|}{|1} + \frac{z^2|}{|3 - z^2} + \frac{9z^2|}{|5 - 3z^2} + \frac{25z^2|}{|7 - 5z^2} + \cdots .$$

When $z = 1$, this becomes what is now viewed as the first infinite continued fraction, given by Lord Brouncker (1620–1684):

$$\frac{4}{\pi} = 1 + \frac{1|}{|2} + \frac{3^2|}{|2} + \frac{5^2|}{|2} + \frac{7^2|}{|2} + \frac{9^2|}{|2} + \cdots . \tag{9.8}$$

Brouncker intuited this result from Stirling's work on the factorial.

Exercise 9.7 (see also [74]) Legitimate the derivation of Brouncker's irregular fraction (9.8) for $4/\pi$.

Furthermore, since

$$\arctan z = \frac{\log(1 + iz) - \log(1 - iz)}{2i},$$

we also obtain a variant of Euler's continued fraction for $\log((1 + z)/(1 - z))$.

Exercise 9.8 ([74]) Find the value of the continued fraction

$$\frac{1|}{|1} + \frac{1^2|}{|1} + \frac{2^2|}{|1} + \frac{3^2|}{|1} + \frac{4^2|}{|1} + \frac{5^2|}{|1} + \cdots .$$

While elegant, Euler's continued fraction is much less useful than that of Gauss, to which we now turn.

9.3 Gauss continued fraction for the hypergeometric function

A classical result on an irregular continued fraction for the so-called *hypergeometric function* goes back to Gauss. The function is defined by the series

$$\begin{aligned} F(a,b;c;z) &= \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{n!(c)_n} z^n \\ &= 1 + \frac{a \times b}{1 \times c} z + \frac{a(a+1) \times b(b+1)}{1 \times 2 \times c(c+1)} z^2 \\ &\quad + \frac{a(a+1)(a+2) \times b(b+1)(b+2)}{1 \times 2 \times 3 \times c(c+1)(c+2)} z^3 + \cdots, \end{aligned}$$

where the notation

$$(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)} = a(a+1)\cdots(a+n-1)$$

stands for the *Pochhammer symbol* (or *shifted factorial*; note that $(1)_n = n!$). It is not hard to check that the series converges for $|z| < 1$. Among the many properties possessed by the function $F(z) = F(a,b;c;z)$, the fact that it satisfies a second-order linear homogeneous differential equation,

$$z(1-z)\frac{\mathrm{d}^2 F}{\mathrm{d}z^2} + (c - (a+b+1)z)\frac{\mathrm{d}F}{\mathrm{d}z} - abF = 0,$$

is crucial. Using this relation one can efficiently construct the analytic continuation of the function $F(z)$, originally defined by the series above, to the whole complex plane with a branch cut along the real ray $[1, \infty)$.

An important feature of the hypergeometric function (and its generalisations) is that it encompasses many other functions, including elementary ones, as either special or limiting cases. For example,

$$\begin{gathered} \log(1+z) = zF(1,1;2;-z), \qquad (1+z)^{-a} = F(a,b;b;-z), \\ e^z = \lim_{b\to\infty} F(1,b;1,z/b), \qquad \arcsin z = zF(1/2,1/2;3/2;z^2) \\ \text{and} \qquad \arctan z = zF(1,1/2;3/2;-z^2). \end{gathered}$$

Lemma 9.9 *The following* contiguous *relation holds:*

$$F(a,b;c;z) - F(a+1,b;c+1;z) = \frac{(a-c)b}{c(c+1)} zF(a+1,b+1;c+2;z). \quad (9.9)$$

Proof Indeed, we have

$$\begin{aligned}
&F(a,b;c;z) - F(a+1,b;c+1;z)\\
&\quad= \sum_{n=0}^{\infty} \frac{(a)_n(b)_n}{n!(c+1)_n}\left(\frac{c+n}{c} - \frac{a+n}{a}\right) z^n\\
&\quad= \sum_{n=1}^{\infty} \frac{(a)_n(b)_n}{n!(c+1)_n}\, \frac{(a-c)n}{ac}\, z^n\\
&\quad= \sum_{m=0}^{\infty} \frac{(a)_{m+1}(b)_{m+1}}{m!(c+1)_{m+1}}\, \frac{a-c}{ac}\, z^{m+1}\\
&\quad= \frac{(a-c)bz}{c(c+1)} \sum_{m=0}^{\infty} \frac{(a+1)_m(b+1)_m}{m!(c+2)_m}\, z^m. \qquad \square
\end{aligned}$$

Note that, because of the symmetry between a and b in the hypergeometric function $F(a,b;c;z)$, we also obtain from (9.9) another contiguous relation:

$$F(a,b;c;z) - F(a,b+1;c+1;z) = \frac{a(b-c)}{c(c+1)}\, zF(a+1,b+1;c+2;z). \tag{9.10}$$

Theorem 9.10 (Gauss continued fraction) *We have*

$$\frac{F(a+1,b;c+1;z)}{cF(a,b;c;z)} = \frac{1|}{|c} + \frac{\lambda_0 z|}{|c+1} + \frac{\lambda_1 z|}{|c+2} + \cdots + \frac{\lambda_n z|}{|c+n+1} + \cdots, \tag{9.11}$$

where $\lambda_{2k-1} = (a+k)(b-c-k)$ *and* $\lambda_{2k} = (a-c-k)(b+k)$.

Proof For $k = 0, 1, 2, \ldots$, define

$$F_{2k}(z) = F(a+k, b+k; c+2k; z)$$

and

$$F_{2k+1}(z) = F(a+k+1, b+k; c+2k+1; z).$$

Then

$$\begin{aligned}
F_{2k}(z) - F_{2k+1}(z) &= \frac{(a-c-k)(b+k)}{(c+2k)(c+2k+1)}\, zF_{2k+2}(z),\\
F_{2k-1}(z) - F_{2k}(z) &= \frac{(a+k)(b-c-k)}{(c+2k-1)(c+2k)}\, zF_{2k+1}(z),
\end{aligned}$$

by the contiguous relations (9.9) and (9.10), respectively. Therefore

$$\frac{F_{n+1}(z)}{F_n(z)} = \cfrac{1}{1 + \dfrac{\lambda_n z}{(c+n)(c+n+1)}\, \dfrac{F_{n+2}(z)}{F_{n+1}(z)}},$$

where $\lambda_{2k} = (a-c-k)(b+k)$ and $\lambda_{2k-1} = (a+k)(b-c-k)$, so that

$$\frac{F_1(z)}{F_0(z)} = \frac{1|}{|1} + \frac{\frac{\lambda_0 z}{c(c+1)}|}{|1} + \frac{\frac{\lambda_1 z}{(c+1)(c+2)}|}{|1} + \cdots + \frac{\frac{\lambda_n z}{(c+n)(c+n+1)}|}{|1} + \cdots .$$

It remains to pass to the equivalent continued fraction by taking $c_n = c + n - 1$ for $n = 1, 2, \ldots$ in the notation of Theorem 9.5. □

Our derivation of the Gauss continued fraction follows the lines of Section 2.10, where we derived a continued fraction for a confluent hypergeometric function, also known as Bessel's function. By taking the limit $a \to 0$ in (9.11) and specialising to $c = b$, we obtain the continued fraction

$$\begin{aligned}\sum_{n=0}^{\infty} \frac{z^n}{b+n} &= \frac{F(1, b; b+1; z)}{b} \\ &= \frac{1|}{|b} + \frac{\lambda_0' z|}{|b+1} + \frac{\lambda_1' z|}{|b+2} + \cdots + \frac{\lambda_n' z|}{|b+n+1} + \cdots , \end{aligned} \tag{9.12}$$

where $\lambda'_{2k-1} = -k^2$ and $\lambda'_{2k} = -(b+k)^2$; this can be used to construct continued fractions for

$$\log(1+z) = zF(1, 1; 2; -z) \qquad \text{and} \qquad \arctan z = zF(1, 1/2; 3/2; -z^2),$$

as well as for the tails of their power series.

Theorem 9.11 *For $N = 1, 2, \ldots$, we have*

$$\begin{aligned}\log(1+z) - \sum_{n=1}^{N-1} \frac{(-1)^{n-1} z^n}{n} &= \frac{(-1)^{N-1} z^N|}{|N} + \frac{N^2 z|}{|N+1} + \frac{1^2 z|}{|N+2} \\ &\quad + \frac{(N+1)^2 z|}{|N+3} + \frac{2^2 z|}{|N+4} + \cdots , \end{aligned} \tag{9.13}$$

$$\begin{aligned}\arctan z - \sum_{n=0}^{N-1} \frac{(-1)^n z^{2n+1}}{2n+1} &= \frac{(-1)^N z^{2N+1}|}{|2N+1} + \frac{(2N+1)^2 z^2|}{|2N+3} + \frac{2^2 z^2|}{|2N+5} \\ &\quad + \frac{(2N+3)^2 z^2|}{|2N+7} + \frac{4^2 z^2|}{|2N+9} + \cdots . \end{aligned} \tag{9.14}$$

Proof Use

$$\log(1+z) - \sum_{n=1}^{N-1} \frac{(-1)^{n-1} z^n}{n} = \frac{z^N\, F(1, N; N+1; -z)}{N}$$

and

$$\arctan z - \sum_{n=0}^{N-1} \frac{(-1)^n z^{2n+1}}{2n+1} = \frac{z^{2N+1}\, F(1, N+1/2; N+2/2; -z^2)}{2(N+1/2)}$$

together with the continued fraction (9.12). □

Note that further specialisation to $z = 1$ in (9.14) leads to a continued fraction for the tail of the approximation of $\pi/4$ by Gregory's series:

$$\frac{\pi}{4} - \sum_{n=0}^{N-1} \frac{(-1)^n}{2n+1} = \frac{(-1)^N|}{|2N+1} + \frac{(2N+1)^2|}{|2N+3} + \frac{2^2|}{|2N+5} + \frac{(2N+3)^2|}{|2N+7} + \frac{4^2|}{|2N+9} + \cdots, \tag{9.15}$$

while its special case $N = 0$ gives

$$\pi = \frac{4|}{|1} + \frac{1^2|}{|3} + \frac{2^2|}{|5} + \frac{3^2|}{|7} + \cdots + \frac{n^2|}{|2n+1} + \cdots. \tag{9.16}$$

The estimates given in [25, Theorem 4] show that, for large b and z from the range $-1 \le z < 0$, the quality of approximation of the hypergeometric value by the nth convergent from (9.12) is roughly bounded by $(z/(z-1))^n$. The estimate is applicable in the case of (9.15), thus showing that the convergents to the continued fraction can be used to accelerate the convergence of Gregory's series. Note that the paper [25] discusses an interesting phenomenon concerning the tail (9.15) of Gregory's series, which relates to its asymptotic power series in $1/N$ as $N \to \infty$.

Finally, we mention that, on using the Nth convergent of the continued fraction in (9.13) for $z = 1$, it is possible to demonstrate that the resulting rational approximations to $\log 2$ are sufficient for proving the irrationality of the number (using Theorem 1.34) as well as for producing a bound for its irrationality exponent (using Theorem 1.35). We will not pursue this topic further here, but the idea is developed by M. Prévost in [137] for irrationality proofs of the constants $\zeta(2)$ and $\zeta(3)$.

9.4 Ramanujan's AGM continued fraction

In this section we give a taste of Ramanujan's AGM continued fraction; the more famous Rogers–Ramanujan continued fraction is discussed in the chapter notes. The substantial technical details can be found in the papers [26, 27, 19] and [102].

In [26, 27] one of the present authors considered the arithmetic-geometric mean (AGM) fraction, found in Chapter 18 of Ramanujan's *second notebook*

[13]. For $a, b, \eta > 0$ we have

$$\mathcal{R}_\eta(a,b) = \cfrac{a}{\eta + \cfrac{b^2}{\eta + \cfrac{4a^2}{\eta + \cfrac{9b^2}{\eta + \ddots}}}}, \tag{9.17}$$

one of whose remarkable properties is a formal AGM relation that is known to be true at least for positive real a, b:

$$\mathcal{R}_1\left(\frac{a+b}{2}, \sqrt{ab}\right) = \frac{\mathcal{R}_1(a,b) + \mathcal{R}_1(b,a)}{2}. \tag{9.18}$$

However, this relation is of dubious validity for general complex parameters [26] despite claims in the literature. Note that $\mathcal{R}_\eta(a,b) = \mathcal{R}_1(a/\eta, b/\eta)$ and that validity of (9.18) depends only on the ratio a/b, which can be thought as a point of the extended complex field $\overline{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$.

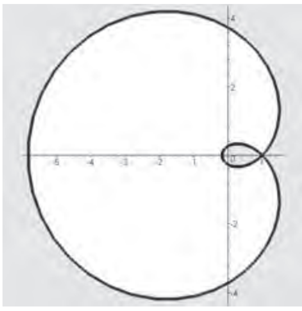

Figure 9.1 Cardioid on whose complement (shaded) AGM relation (9.18) holds.

Work in [27] focused on the convergence domain

$$\mathcal{D}_0 = \{(a,b) \in \mathbb{C}^2 : \mathcal{R}_1(a,b) \text{ converges on } \overline{\mathbb{C}}\}.$$

It was proved therein that, with

$$\mathcal{D}_1 = \{(a,b) \in \mathbb{C}^2 : |a| \neq |b|\} \cup \{(a,b) \in \mathbb{C}^2 : a^2 = b^2 \notin (-\infty, 0)\},$$

we have $\mathcal{D}_1 \subseteq \mathcal{D}_0$, so that the Ramanujan continued fraction converges for almost all complex pairs (a,b). The article [19] showed that $\mathcal{D}_1 = \mathcal{D}_0$. Equivalently, the fraction $\mathcal{R}_1$ diverges whenever $0 \neq a = be^{i\phi}$ with $\cos^2\phi \neq 1$ or $a^2 = b^2 \in (-\infty, 0)$. It was also shown that remarkable and explicit chaotic dynamics occur on the imaginary axis, say for $\mathcal{R}_1(i, i)$. Key to all this analysis is the following theorem, whose components date back to the nineteenth century. The notation

$$\vartheta_2(q) = \sum_{\substack{k\in\mathbb{Z}\\ k \text{ odd}}} q^{k^2/4} = 2q^{1/4}\sum_{n=0}^{\infty} q^{n(n+1)}, \qquad \vartheta_3(q) = \sum_{\substack{k\in\mathbb{Z}\\ k \text{ even}}} q^{k^2/4} = 1 + 2\sum_{n=1}^{\infty} q^{n^2}$$

stands for the classical theta (null) functions [166].

Theorem 9.12 ([26, 19]) *For real $y, \eta > 0$ and $q = e^{-\pi y}$, we have the theta function parametrisations*

$$\eta \sum_{\substack{k\in\mathbb{Z}\\ k \text{ odd}}} \frac{\operatorname{sech}(k\pi y/2)}{\eta^2 + k^2} = \mathcal{R}_\eta(\vartheta_2^2(q), \vartheta_3^2(q)),$$
$$\eta \sum_{\substack{k\in\mathbb{Z}\\ k \text{ even}}} \frac{\operatorname{sech}(k\pi y/2)}{\eta^2 + k^2} = \mathcal{R}_\eta(\vartheta_3^2(q), \vartheta_2^2(q)).$$

Moreover, the equality (9.18) *holds when a/b belongs to the closed exterior of the cardioid knot shown in Figure* 9.1*, which in polar coordinates is given by* $r^2 + (2\cos\phi - 4)r + 1 = 0$.

Interpreting Theorem 9.12 as giving a Riemann integral in the limit $b \to a^-$ (for $a > 0$), gives a slew of relations involving the *psi* or *digamma* function

$$\psi(z) = \frac{\mathrm{d}}{\mathrm{d}z}\log\Gamma(z),$$

the hypergeometric function and the Gauss continued fraction (see Section 9.3).

Corollary 9.13 ([26]) *For all $a > 0$,*

$$\begin{aligned}
\mathcal{R}_1(a, a) &= \int_0^\infty \frac{\operatorname{sech}(\pi x/(2a))}{1 + x^2}\,\mathrm{d}x \\
&= 2a\sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{1 + (2k-1)a} \\
&= \frac{1}{2}\left(\psi\left(\frac{3}{4} + \frac{1}{4a}\right) - \psi\left(\frac{1}{4} + \frac{1}{4a}\right)\right) \\
&= \frac{2a}{1+a}\,F\left(\frac{1}{2a} + \frac{1}{2}, 1; \frac{1}{2a} + \frac{3}{2}; -1\right) \\
&= 2\int_0^1 \frac{t^{1/a}}{1 + t^2}\,\mathrm{d}t \\
&= \int_0^\infty e^{-x/a}\operatorname{sech} x\,\mathrm{d}x.
\end{aligned}$$

No closed form is known for any case with $a \neq b$. In [29, 30] various extensions were studied and fractions with period 3 and other features were elaborated.

Exercise 9.14 Derive a restricted parametrised form of (9.18) from Theorem 9.12 (as $q \mapsto q^2$).

Exercise 9.15 Derive Corollary 9.13 from Theorem 9.12.

Hint The expressions are listed in an order suited to proving each expression from the previous one. □

Exercise 9.16 ([26]) Use Corollary 9.13 to determine that $\mathcal{R}_1(1,1) = \log 2$ and $\mathcal{R}_1(1/2,1/2) = 2 - \pi/2$. Obtain for positive integers p, q that

$$\begin{aligned}\mathcal{R}_1\left(\frac{p}{q},\frac{p}{q}\right) &= -2p\sum_{n=1}^{p+q-1}\frac{1}{n}\left(\delta_{n\equiv p+q \pmod{4p}} - \delta_{n\equiv 3p+q \pmod{4p}}\right)\\ &\quad - 2\sum_{\substack{0<k<2p\\ k\text{ odd}}}\cos\frac{(p+q)k\pi}{2p}\,\log\left(2\sin\frac{k\pi}{4p}\right)\\ &\quad + 2\pi\sum_{\substack{0<k<2p\\ k\text{ odd}}}\left(\frac{1}{2}-\frac{k}{4p}\right)\sin\frac{(p+q)k\pi}{2p},\end{aligned}$$

where δ_X denotes the indicator of set X.

The convergence of (9.17) is slowest – at an arithmetic rate – when $a = b$. The key to analysing the AGM fraction is the replacement of the irregular fraction by a *reduced continued fraction*, in which, as observed earlier, we have the same form as in a regular fraction except that we require that a_n be real or complex.

Exercise 9.17 Show that for all a, b we have

$$\mathcal{R}_1(a,b) = \frac{a}{[a_1, a_2, \ldots, a_n, \ldots]},$$

where

$$\begin{aligned} a_n &= \frac{n!^2}{(n/2)!^4}\,4^{-n}\,\frac{b^n}{a^n} \approx \frac{2}{\pi n}\,\frac{b^n}{a^n} && \text{for even } n,\\ a_n &= \frac{((n-1)/2)!^4}{n!^2}\,4^{n-1}\,\frac{a^{n-1}}{b^{n+1}} \approx \frac{\pi}{2abn}\,\frac{a^n}{b^n} && \text{for odd } n,\end{aligned}$$

and so the series $\sum_{n=1}^{\infty} a_n$ diverges.

Now, the Seidel–Stern theorem [82, 103] asserts that for reduced fractions with positive terms the sum diverges iff the fraction converges. This shows that for real $a, b > 0$ the continued fraction $\mathcal{R}_1(a,b)$ converges.

Effective algorithms for computing (9.17) in the full complex plane are given in [26, 27]. They produce D good digits for $O(D)$ operations where the order constant D is independent of a, b, η.

9.5 An irregular continued fraction for $\zeta(2) = \pi^2/6$

Recall the definition of the Riemann zeta function from (1.8). In this section we will construct an irregular continued fraction for the number

$$\zeta(2) = \sum_{n=1}^{\infty} \frac{1}{n^2}.$$

The fact that $\zeta(2) = \pi^2/6$ is known from analysis. For example, it follows from the Fourier expansion of the function x^2 or from the product formula for the function $\sin x$; see [157, 28].

Exercise 9.18 ([28]) Show by elementary methods that

$$\left(\sum_{n=-\infty}^{\infty} \frac{(-1)^n}{2n+1} \right)^2 = \sum_{n=-\infty}^{\infty} \frac{1}{(2n+1)^2}.$$

Deduce from this that $\zeta(2) = \pi^2/6$.

Hint Let

$$\delta_N = \sum_{m,n=-N}^{N} \frac{(-1)^{n+m}}{(2n+1)(2m+1)} - \sum_{k=-N}^{N} \frac{1}{(2k+1)^2} \qquad \text{and} \qquad \varepsilon_N = \sum_{\substack{m,n=-N \\ m \neq n}}^{N} \frac{1}{m-n}.$$

Show that $\varepsilon_N \leq 1/(N-n+1)$, while

$$\delta_N = \sum_{\substack{m,n=-N \\ m \neq n}}^{N} \frac{(-1)^{n+m}}{(2n+1)(m-n)} \to 0. \qquad \square$$

For each $n = 0, 1, 2, \ldots$, define the rational function

$$R_n(t) = (-1)^n \frac{n! \prod_{j=1}^{n} (t-j)}{\prod_{j=0}^{n} (t+j)^2}$$

and consider the quantity

$$r_n = \sum_{\nu=1}^{\infty} R_n(\nu).$$

The latter series converges (absolutely), since $R_n(t) = O(t^{-2})$ as $t \to \infty$.

Lemma 9.19 *The following representation holds:*

$$r_n = q_n\zeta(2) - p_n, \qquad n = 0, 1, 2, \dots,$$

where

$$q_n = \sum_{k=0}^{n} \big(R_n(t)(t+k)^2\big)\Big|_{t=-k} \in \mathbb{Q} \qquad \textit{and} \qquad p_n \in \mathbb{Q}, \qquad n = 0, 1, 2, \dots$$

In addition, for $n = 0$ *and* $n = 1$ *we have* $r_0 = \zeta(2)$ *and* $r_1 = 3\zeta(2) - 5$*, that is,*

$$p_0 = 0, \quad q_0 = 1 \qquad \textit{and} \qquad p_1 = 5, \quad q_1 = 3.$$

Proof First, consider the particular cases $n = 0$ and $n = 1$. For $n = 0$ we have $R_0(t) = 1/t^2$, and hence

$$r_0 = \sum_{\nu=1}^{\infty} R_0(\nu) = \zeta(2).$$

For $n = 1$ we decompose the function $R_1(t)$ into a sum of partial fractions:

$$R_1(t) = -\frac{t-1}{t^2(t+1)^2} = \frac{1}{t^2} + \frac{2}{(t+1)^2} - \frac{3}{t} + \frac{3}{t+1}.$$

Thus,

$$\begin{aligned} r_1 &= \sum_{\nu=1}^{\infty} R_1(\nu) = \sum_{\nu=1}^{\infty} \Big(\frac{1}{t^2} + \frac{2}{(t+1)^2} - \frac{3}{t} + \frac{3}{t+1}\Big) \\ &= \sum_{\nu=1}^{\infty} \frac{1}{\nu^2} + \sum_{\nu=2}^{\infty} \frac{2}{\nu^2} + \sum_{\nu=1}^{\infty} \Big(\frac{3}{\nu+1} - \frac{3}{\nu}\Big) \\ &= \zeta(2) + 2(\zeta(2) - 1) - 3 = 3\zeta(2) - 5. \end{aligned}$$

In the general case, let us replace the quantity r_n with the power series

$$r_n(z) = \sum_{\nu=1}^{\infty} R_n(\nu)\, z^{\nu},$$

which converges at $z = 1$ by the argument indicated above. The partial-fraction decomposition of $R_n(t)$ is as follows:

$$R_n(t) = \sum_{k=0}^{n} \Big(\frac{A_k}{(t+k)^2} + \frac{B_k}{t+k}\Big),$$

where A_k and B_k are certain rational numbers. For the moment, we need 'explicit' formulae for the coefficients

$$A_k = \big(R_n(t)(t+k)^2\big)\Big|_{t=-k}, \qquad k = 0, 1, \dots, n,$$

only. We obtain

$$\begin{aligned} r_n(z) &= \sum_{\nu=1}^{\infty} R_n(\nu)\, z^\nu = \sum_{\nu=1}^{\infty}\sum_{k=0}^{n} \frac{A_k\, z^\nu}{(\nu+k)^2} + \sum_{\nu=1}^{\infty}\sum_{k=0}^{n} \frac{B_k\, z^\nu}{\nu+k} \\ &= \sum_{k=0}^{n} A_k\, z^{-k} \sum_{\nu=1}^{\infty} \frac{z^{\nu+k}}{(\nu+k)^2} + \sum_{k=0}^{n} B_k\, z^{-k} \sum_{\nu=1}^{\infty} \frac{z^{\nu+k}}{\nu+k} \\ &= \sum_{k=0}^{n} A_k\, z^{-k}\Big(\sum_{l=1}^{\infty}\frac{z^l}{l^2} - \sum_{l=1}^{k}\frac{z^l}{l^2}\Big) + \sum_{k=0}^{n} B_k\, z^{-k}\Big(\sum_{l=1}^{\infty}\frac{z^l}{l} - \sum_{l=1}^{k}\frac{z^l}{l}\Big) \\ &= A(z)\sum_{l=1}^{\infty}\frac{z^l}{l^2} + B(z)\sum_{l=1}^{\infty}\frac{z^l}{l} - C(z) \\ &= A(z)\sum_{l=1}^{\infty}\frac{z^l}{l^2} + B(z)(-\log(1-z)) - C(z), \end{aligned}$$

where

$$A(z) = \sum_{k=0}^{n} A_k\, z^{-k} \in \mathbb{Q}[z^{-1}], \qquad B(z) = \sum_{k=0}^{n} B_k\, z^{-k} \in \mathbb{Q}[z^{-1}],$$

$$C(z) = \sum_{k=0}^{n} A_k\, z^{-k} \sum_{l=1}^{k} \frac{z^l}{l^2} + \sum_{k=0}^{n} B_k\, z^{-k} \sum_{l=1}^{k} \frac{z^l}{l} \in \mathbb{Q}[z^{-1}].$$

Since the power series $r_n(z)$ converges at $z = 1$, we can use Abel's theorem, which says that the right-hand side of the resulting series $r_n(z)$ has a finite limit r_n as $z \to 1$. In particular, this means that $B(1) = 0$ and $r_n = r_n(1) = A(1)\zeta(2) - C(1)$. It remains to take $q_n = A(1) = \sum_{k=0}^{n} A_k$ and $p_n = C(1)$. □

Note that the function $R_{n+1}(t)/R_n(t)$ is a rational function not only of the parameter t but also of n. Let us define another (rational) function $S_n(t) = s_n(t)R_n(t)$, where

$$s_n(t) = 11n^2 + 9n + 2 + 3(2n+1)t - t^2. \tag{9.19}$$

Lemma 9.20 *For each integer $n = 1, 2, \dots,$ the following identity holds:*

$$(n+1)^2 R_{n+1}(t) - (11n^2 + 11n + 3)R_n(t) - n^2 R_{n-1}(t) = S_n(t+1) - S_n(t). \tag{9.20}$$

Proof Since

$$\frac{R_{n-1}(t)}{R_n(t)} = -\frac{(t+n)^2}{n(t-n)}, \qquad \frac{R_{n+1}(t)}{R_n(t)} = -\frac{(n+1)(t-n-1)}{(t+n+1)^2},$$

$$\frac{S_n(t+1)}{R_n(t)} = \frac{S_n(t+1)}{R_n(t+1)}\,\frac{R_n(t+1)}{R_n(t)} = s_n(t+1)\frac{t^3}{(t-n)(t+n+1)^2},$$

the proof is reduced to verification of the identity

$$(n+1)^2\Big(-\frac{(n+1)(t-n-1)}{(t+n+1)^2}\Big)-(11n^2+11n+3)-n^2\Big(-\frac{(t+n)^2}{n(t-n)}\Big)$$
$$= s_n(t+1)\frac{t^3}{(t-n)(t+n+1)^2}-s_n(t), \tag{9.21}$$

where the polynomial $s_n(t)$ is given in (9.19). Calculation shows that both sides of (9.21) are equal to

$$\frac{\xi_n(t)}{(t-n)(t+n+1)^2}$$

where

$$\xi_n(t) = nt^4-(7n^2+9n+3)t^3-(6n^3+30n^2+27n+7)t^2$$
$$+(17n^4+24n^3+3n^2-6n-2)t+(11n^4+31n^3+31n^2+13n+2)n. \quad \square$$

Theorem 9.21 *The sequences $(r_n)_{n=0}^{\infty}$, $(q_n)_{n=0}^{\infty}$ and $(p_n)_{n=0}^{\infty}$ each satisfy the recurrence relation*

$$(n+1)^2r_{n+1}-(11n^2+11n+3)r_n-n^2r_{n-1}=0, \qquad n=1,2,\dots \tag{9.22}$$

Proof We use the definition of r_n and Lemma 9.20: thus,

$$(n+1)^2r_{n+1}-(11n^2+11n+3)r_n-n^2r_{n-1}$$
$$=\sum_{\nu=1}^{\infty}(S_n(t+1)-S_n(t))\Big|_{t=\nu}=-S_n(1)=-s_n(1)\,R_n(1)=0,$$

because $R_n(1)=0$ for $n=1,2,\dots$

For the sequence of coefficients q_n, we use the formula from the proof of Lemma 9.19:

$$q_n=\sum_{k=0}^{n}(R_n(t)(t+k)^2)\Big|_{t=-k}=\sum_{k\in\mathbb{Z}}(R_n(t)(t+k)^2)\Big|_{t=-k},$$

where we have $(R_n(t)(t+k)^2)\big|_{t=-k}=0$ for $k<0$ and $k>n$ for trivial reasons. With the help of identity (9.20) we find that

$$(n+1)^2q_{n+1}-(11n^2+11n+3)q_n-n^2q_{n-1}$$
$$=\sum_{k\in\mathbb{Z}}((S_n(t+1)-S_n(t))(t+k)^2)\Big|_{t=-k}$$
$$=\sum_{k\in\mathbb{Z}}((S_n(l-k+1)-S_n(l-k))l^2)\Big|_{l=0}$$
$$=\Big(l^2\sum_{k\in\mathbb{Z}}(S_n(l-k+1)-S_n(l-k))\Big)\Big|_{l=0}=0$$

for $n = 0, 1, 2, \ldots$, since the inner sum over k telescopes.

Finally, the sequence $p_n = q_n\zeta(2) - r_n$ satisfies the required recurrence as a linear combination (with constant coefficients) of the sequences q_n and r_n. □

Lemma 9.22 *For all $n = 0, 1, 2, \ldots$ we have $q_n \geq 1$. Moreover, $r_n \to 0$ as $n \to \infty$.*

Proof From Lemma 9.19 we have $q_0 = 1$ and $q_1 = 3 > 1$. Hence an inductive argument gives us

$$q_{n+1} = \frac{(11n^2 + 11n + 3)q_n + n^2 q_{n-1}}{(n+1)^2} \geq \frac{(11n^2 + 11n + 3) + n^2}{(n+1)^2} > 1$$

for $n = 1, 2, \ldots$ The fact that $r_n \to 0$ as $n \to \infty$ (indeed, a stronger statement than that about the asymptotics of the quantities r_n) will be proved in the next section. □

As a consequence, we derive that

$$\frac{p_n}{q_n} = \zeta(2) - \frac{r_n}{q_n} \to \zeta(2) \qquad \text{as } n \to \infty. \tag{9.23}$$

Thus, we have constructed a sequence of *rational* numbers $(p_n)_{n=0}^{\infty}$ and $(q_n)_{n=0}^{\infty}$ that satisfy the recurrence relation

$$p_n = \frac{P(n-1)}{n^2} p_{n-1} + \frac{(n-1)^2}{n^2} p_{n-2},$$
$$q_n = \frac{P(n-1)}{n^2} q_{n-1} + \frac{(n-1)^2}{n^2} q_{n-2},$$

where $P(n) = 11n^2 + 11n + 3$, for $n = 2, 3, \ldots$ Setting $p_{-1} = 1$, $q_{-1} = 0$ and taking into account that $p_0 = 0$, $q_0 = 1$ and $p_1 = 5$, $q_1 = 3$, by Lemma 9.19, we conclude that

$$p_1 = 3p_0 + 5p_{-1}, \qquad q_1 = 3q_0 + 5q_{-1}.$$

We are now in a position to apply Theorem 9.1. The continued fraction given by

$$\frac{b_1|}{|a_1} + \frac{b_2|}{|a_2} + \frac{b_3|}{|a_3} + \cdots + \frac{b_n|}{|a_n} + \cdots,$$

$$\text{with} \qquad a_n = \frac{P(n-1)}{n^2} \quad \text{for } n = 1, 2, \ldots, \tag{9.24}$$
$$b_1 = 5, \quad b_n = \frac{(n-1)^2}{n^2} \quad \text{for } n = 2, 3, \ldots,$$

has $(p_n)_{n=-1}^{\infty}$ and $(q_n)_{n=-1}^{\infty}$ as the sequences of numerators and denominators of its convergents; moreover, we have $p_n/q_n \to \zeta(2)$ as $n \to \infty$ by (9.23). Hence

$\zeta(2)$ is the value of the continued fraction (9.24). Developing the equivalent transformation of the resulted continued fraction (see Theorem 9.5) with the choices $c_0 = 1$ and $c_n = n^2$ for $n = 1, 2, \dots$, we finally arrive at the continued fraction

$$\zeta(2) = \frac{b'_1|}{|a'_1} + \frac{b'_2|}{|a'_2} + \frac{b'_3|}{|a'_3} + \cdots + \frac{b'_n|}{|a'_n} + \cdots$$

$$\text{with} \qquad a'_n = P(n-1) \quad \text{for } n = 1, 2, \dots,$$

$$b'_1 = 5, \quad b'_n = (n-1)^4 \quad \text{for } n = 2, 3, \dots$$

Let us summarise our findings in the following statement.

Theorem 9.23 *We have the following (irregular) continued fraction:*

$$\zeta(2) = \frac{5|}{|3} + \frac{1^4|}{|P(1)} + \frac{2^4|}{|P(2)} + \cdots + \frac{n^4|}{|P(n)} + \cdots,$$

where $P(n) = 11n^2 + 11n + 3$.

Exercise 9.24 (Irregular continued fraction for $\zeta(3)$) Take the rational function

$$\tilde{R}_n(t) = \frac{\prod_{j=1}^{n}(t-j)^2}{\prod_{j=0}^{n}(t+j)^2}$$

and, for each $n = 0, 1, 2, \dots$, consider the (absolutely convergent) series

$$\tilde{r}_n = -\sum_{\nu=1}^{\infty} \frac{\mathrm{d}\tilde{R}_n(t)}{\mathrm{d}t}\bigg|_{t=\nu}.$$

(a) Show that

$$\tilde{r}_0 = 2\zeta(3) \qquad \text{and} \qquad \tilde{r}_1 = 10\zeta(3) - 12.$$

(b) Show that, for each $n = 0, 1, 2, \dots$, we have $\tilde{r}_n = \tilde{q}_n\zeta(3) - \tilde{p}_n$, where $\tilde{p}_n$ and $\tilde{q}_n$ are rational numbers, $\tilde{q}_n > 0$.

(c) Define $\tilde{S}_n(t) = \tilde{s}_n(t)\tilde{R}_n(t)$, where

$$\tilde{s}_n(t) = 4(2n+1)(-2t^2 + t + (2n+1)^2).$$

Check that

$$(n+1)^3\tilde{R}_{n+1}(t) - (2n+1)(17n^2 + 17n + 5)\tilde{R}_n(t) + n^3\tilde{R}_{n-1}(t) = \tilde{S}_n(t+1) - \tilde{S}_n(t) \tag{9.25}$$

for $n = 1, 2, \dots$

(d) Using (c), show that the sequences $(\tilde{r}_n)_{n=0}^{\infty}$, $(\tilde{q}_n)_{n=0}^{\infty}$ and $(\tilde{p}_n)_{n=0}^{\infty}$ each satisfy the recurrence relation

$$(n+1)^3\tilde{r}_{n+1} - (2n+1)(17n^2+17n+5)\tilde{r}_n + n^3\tilde{r}_{n-1} = 0, \qquad n = 1, 2, \ldots \tag{9.26}$$

(e) Assuming that $\tilde{r}_n \to 0$ as $n \to \infty$, prove the following continued fraction expansion for $\zeta(3)$:

$$\zeta(3) = \frac{6|}{|5} + \frac{-1^6|}{|Q(1)} + \frac{-2^6|}{|Q(2)} + \cdots + \frac{-n^6|}{|Q(n)} + \cdots,$$

where $Q(n) = (2n+1)(17n^2+17n+5)$.

9.6 The irrationality of π^2

The aim of this final section is to prove that $\zeta(2)$ is irrational.

Theorem 9.25 *The number $\zeta(2) = \pi^2/6$ is irrational.*

The proof, which we present below, is based on the original construction of Apéry (who also proved the irrationality of $\zeta(3)$; see Exercises 9.24 and 9.30). However, our ideas considerably differ from those of Apéry. Note that the irrationality problem of the numbers $\zeta(5), \zeta(7), \zeta(9), \ldots$ is not yet resolved.

As in the previous section, to each $n = 0, 1, 2, \ldots$ we assign the rational function

$$R_n(t) = (-1)^n \frac{n! \prod_{j=1}^{n}(t-j)}{\prod_{j=0}^{n}(t+j)^2}$$

and the corresponding quantity

$$r_n = \sum_{\nu=1}^{\infty} R_n(\nu) = q_n\zeta(2) - p_n.$$

Let $d_n = \operatorname{lcm}(1, 2, \ldots, n)$. The corollary of the prime number theorem (see Theorem 1.20) asserts that

$$\lim_{n\to\infty} \frac{\log d_n}{n} = 1; \tag{9.27}$$

in other words, that d_n grows with n as $e^{n+o(n)}$.

Lemma 9.26 *The rational coefficients in the partial-fraction decomposition*

$$R_n(t) = \sum_{k=0}^{n}\left(\frac{A_k}{(t+k)^2} + \frac{B_k}{t+k}\right)$$

satisfy the inclusions $A_k \in \mathbb{Z}$ *and* $d_n B_k \in \mathbb{Z}$ *for* $k = 0, 1, \ldots, n$.

Proof Write $R_n(t)$ as a product of two 'simpler' rational functions,

$$R'(t) = \frac{n!}{\prod_{j=0}^{n}(t+j)} = \sum_{k=0}^{n} \frac{A'_k}{t+k}$$

and

$$R''(t) = \frac{(-1)^n \prod_{j=1}^{n}(t-j)}{\prod_{j=0}^{n}(t+j)} = \sum_{k=0}^{n} \frac{A''_k}{t+k}.$$

Then

$$\left.\begin{aligned} A'_k &= \frac{n!}{(-1)^k k!(n-k)!} = (-1)^k \binom{n}{k} \in \mathbb{Z}, \\ A''_k &= \frac{(n+k)!/k!}{(-1)^k k!(n-k)!} = (-1)^k \binom{n}{k}\binom{n+k}{k} \in \mathbb{Z}, \end{aligned}\right\} \qquad k = 0, 1, \ldots, n,$$

whence

$$\begin{aligned} R_n(t) = R'(t)R''(t) &= \sum_{k=0}^{n} \frac{A'_k A''_k}{(t+k)^2} + \sum_{k=0}^{n} \sum_{\substack{l=0 \\ k \neq l}}^{n} \frac{A'_k A''_l}{(t+k)(t+l)} \\ &= \sum_{k=0}^{n} \frac{A'_k A''_k}{(t+k)^2} + \sum_{k=0}^{n} \sum_{\substack{l=0 \\ k \neq l}}^{n} \frac{A'_k A''_l}{l-k}\left(\frac{1}{t+k} - \frac{1}{t+l}\right), \end{aligned}$$

implying that

$$\left.\begin{aligned} A_k &= A'_k A''_k = \binom{n}{k}^2 \binom{n+k}{k}, \\ B_k &= \sum_{\substack{l=0 \\ l \neq k}}^{n} \frac{A'_k A''_l - A'_l A''_k}{l-k}, \end{aligned}\right\} \qquad k = 0, 1, \ldots, n.$$

Since $|l-k| \leq n$ in the last sum, the resulting formulae for A_k and B_k give us grounds for the required inclusions. □

Lemma 9.27 *The rational coefficients of the linear form* $r_n = q_n\zeta(2) - p_n$ *satisfy* $q_n \in \mathbb{Z}$ *and* $d_n^2 p_n \in \mathbb{Z}$.

In other words, the sequence

$$q_n = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}, \qquad n = 0, 1, 2, \ldots,$$

which satisfies the recurrence relation

$$(n+1)^2 q_{n+1} - (11n^2 + 11n + 3)q_n - n^2 q_{n-1} = 0,$$

is *integer-valued*.

Proof In accordance with the formulae from the proof of Lemma 9.19, we have

$$q_n = \sum_{k=0}^{n} A_k, \qquad p_n = \sum_{k=0}^{n} A_k \sum_{l=1}^{k} \frac{1}{l^2} + \sum_{k=0}^{n} B_k \sum_{l=1}^{k} \frac{1}{l}.$$

Using the inclusions of Lemma 9.26 as well as

$$d_n \cdot \sum_{l=1}^{k} \frac{1}{l} \in \mathbb{Z} \quad \text{and} \quad d_n^2 \cdot \sum_{l=1}^{k} \frac{1}{l^2} \in \mathbb{Z} \qquad \text{for } k = 0, 1, \ldots, n,$$

we arrive at the desired claim. □

Lemma 9.28 *For each $n = 1, 2, \ldots$, the following estimate holds:*

$$0 < |r_n| < \frac{7n}{10^n}.$$

Proof Let us estimate the product $M = m(m+1)\cdots(m+n-1)$ of n successive positive integers. As in the proof of Lemma 2.59, we have

$$\int_{m-1}^{m+n-1} \log x \, \mathrm{d}x < \log M = \sum_{l=m}^{m+n-1} \log l < \int_{m}^{m+n} \log x \, \mathrm{d}x$$

implying that

$$\log M > (x \log x - x)\Big|_{x=m-1}^{m+n-1} = \log \frac{(m+n-1)^{m+n-1} e^{-n}}{(m-1)^{m-1}},$$
$$\log M < (x \log x - x)\Big|_{x=m}^{m+n} = \log \frac{(m+n)^{m+n} e^{-n}}{m^m}.$$

Thus,

$$n! < \frac{(n+1)^{n+1} e^{-n}}{1^1}, \qquad \prod_{j=1}^{n} (\nu - j) < \frac{\nu^\nu e^{-n}}{(\nu - n)^{\nu - n}},$$
$$\prod_{j=1}^{n} (\nu + j) > \frac{(\nu + n)^{\nu + n} e^{-n}}{\nu^\nu}$$

for $\nu \ge n+1$; hence

$$\begin{aligned} 0 < (-1)^n R_n(\nu) &< \frac{(n+1)^{n+1}}{\nu^2 n^n} \, \frac{n^n \nu^{3\nu}}{(\nu-n)^{\nu-n}(\nu+n)^{2(\nu+n)}} \\ &= \frac{n}{\nu^2}\Big(1+\frac{1}{n}\Big)^{n+1} \frac{(\nu/n)^{3\nu}}{(\nu/n-1)^{\nu-n}(\nu/n+1)^{2(\nu+n)}} \\ &< \frac{4n}{\nu^2} \, f\Big(\frac{\nu}{n}\Big)^n, \end{aligned}$$

where

$$f(x) = \frac{x^{3x}}{(x-1)^{x-1}(x+1)^{2(x+1)}}.$$

Let C stand for the maximum of the function $f(x)$ in the interval $x > 1$. Then

$$0 < (-1)^n R_n(\nu) < \frac{4n}{\nu^2} C^n,$$

implying that

$$0 < (-1)^n r_n < 4nC^n \sum_{\nu=n+1}^{\infty} \frac{1}{\nu^2} \le 4\zeta(2) n C^n < 7nC^n.$$

It remains to compute the maximum C. We have

$$\begin{aligned} \frac{f'(x)}{f(x)} &= \frac{d}{dx}(3x\log x - (x-1)\log(x-1) - 2(x+1)\log(x+1)) \\ &= 3\log x - \log(x-1) - 2\log(x+1) = \log\frac{x^3}{(x-1)(x+1)^2}; \end{aligned}$$

hence $f'(x) = 0$ if $x^3 = (x-1)(x+1)^2$. A unique root of the latter quadratic equation $-x^2 + x + 1 = 0$ in the interval $x > 1$ is equal to $x_0 = (1+\sqrt{5})/2$. Therefore,

$$\begin{aligned} C = f(x_0) &= \frac{x_0^{3x_0}}{(x_0-1)^{x_0-1}(x_0+1)^{2(x_0+1)}} \\ &= \frac{x_0-1}{(x_0+1)^2}\Big(\frac{x_0^3}{(x_0-1)(x_0+1)^2}\Big)^{x_0} \\ &= \frac{(1+\sqrt{5})/2-1}{((1+\sqrt{5})/2+1)^2} \times 1 = \Big(\frac{\sqrt{5}-1}{2}\Big)^5 < \frac{1}{10}. \end{aligned}$$

This completes our proof of the lemma. □

REMARK 9.29 Dividing both sides of the linear recurrence relation of Theorem 9.21 by n^2, we see that the 'limiting' form of the recurrence for the sequences $(r_n)_{n=0}^{\infty}$, $(q_n)_{n=0}^{\infty}$ and $(p_n)_{n=0}^{\infty}$ is the difference equation

$$r_{n+1} - 11r_n - r_{n-1} = 0$$

with *constant* coefficients. By Theorem 1.27 a general solution of this equation has the form $r_n = c_1\lambda_1^n + c_2\lambda_2^n$, where $c_1, c_2 \in \mathbb{R}$, while $\lambda_1 = ((1-\sqrt{5})/2)^5$ and $\lambda_2 = ((1+\sqrt{5})/2)^5$ are the roots of characteristic polynomial $\lambda^2 - 11\lambda - 1 = 0$. A consequence of the general formula for r_n is the following limit:

$$\lim_{n\to\infty} \sqrt[n]{|r_n|} = \begin{cases} |\lambda_2| & \text{if } c_2 \neq 0; \\ |\lambda_1| & \text{if } c_2 = 0 \text{ and } c_1 \neq 0. \end{cases}$$

Our original difference equation does not have constant coefficients, which constitutes a natural obstacle to obtaining a simple formula for a general solution. However, the limiting relation

$$\limsup_{n\to\infty} \sqrt[n]{|r_n|} \in \{|\lambda_1|, |\lambda_2|\} \tag{9.28}$$

continues to hold whenever r_n is a nontrivial solution. This fact is a classical theorem from analysis due to Poincaré; its proof is not difficult but rather technical [66, Chapter V].

The reasonableness of Poincaré's theorem derives, in part, from its validity for difference equations with constant coefficients (which follows from Theorem 1.27).

Elementary estimation shows that $\limsup_{n\to\infty} \sqrt[n]{|r_n|} \leq 1$; hence, using (9.28), we obtain $\limsup_{n\to\infty} \sqrt[n]{|r_n|} = |\lambda_1| < 1/10$. Thus, Poincaré's theorem could save us from the involved computation in the proof of Lemma 9.28.

Proof of Theorem 9.25 Suppose that, on the contrary, that $\zeta(2) = a/b$, where a and b are certain positive integers. For each $n = 0, 1, 2, \ldots$, the number

$$r_n^* = bd_n^2|r_n| = (-1)^n(d_n^2 q_n a - d_n^2 p_n b)$$

is an integer satisfying $0 < r_n^* < 7nbd_n^2(1/10)^n$. Clearly $r_n \geq 1$, while (9.27) yields $7nbd_n^2 < 3^{2n}$ for all sufficiently large n. The resulting estimate $1 \leq r_n^* < (9/10)^n$ is a contradiction, and proves the theorem. □

Exercise 9.30 Assume the notation of Exercise 9.24.

(a) Show that, for each $n = 0, 1, \ldots$, at least one of $\tilde{r}_n$ and $\tilde{r}_{n+1}$ is nonzero; in other words, the sequence $(\tilde{r}_n)_{n=0}^{\infty}$ is a *nontrivial* solution of the difference equation from Exercise 9.24(d).

(b) Using Poincaré's theorem, verify that

$$\limsup_{n\to\infty} \sqrt[n]{|\tilde{r}_n|} \in \{(\sqrt{2}-1)^4, (\sqrt{2}+1)^4\}.$$

(c) Show, by an elementary estimation, that $|\tilde{r}_n| < Cn$ for a certain constant $C > 0$.

(d) Deduce from (a)–(c) that

$$\limsup_{n\to\infty} \sqrt[n]{|\tilde{r}_n|} = (\sqrt{2}-1)^4 < \frac{4}{3^3 \times 5}.$$

(e) Show that the coefficients of the linear form $\tilde{r}_n = \tilde{q}_n \zeta(3) - \tilde{p}_n$ satisfy $\tilde{q}_n \in \mathbb{Z}$ and $d_n^3 \tilde{p}_n \in \mathbb{Z}$ for $n = 0, 1, 2, \dots$

(f) Deduce from (d) and (e) that $\zeta(3)$ is irrational.

Notes

Throughout this chapter and the rest of this book there lies an iceberg of computation, symbolic and numeric, most of which has not been directly exposed to the reader. The reader would be well advised to keep a computer algebra package open and to implement as much as she or he can! The writers certainly had to use such methods to check or develop many of the more subtle results presented in the book.

One should not miss reading the historical-mathematical account of Apéry's proof [8] of the irrationality of $\zeta(2)$ and $\zeta(3)$ given by Alf van der Poorten in [127]. Our proofs in Sections 9.5 and 9.6 produce Apéry's rational approximations to $\zeta(2)$ (and $\zeta(3)$) but use a somewhat different approach; see [16, 137] for other proofs. It is now apparent that the original construction of Apéry was highly influenced [7, 138] by a continued fraction given by Ramanujan. It should be mentioned that Ramanujan was an indefatigable producer of explicit and highly nontrivial continued fraction expansions, which one could easily classify as beautiful.

Here we limit ourselves to recording the Rogers–Ramanujan continued fractions: for $|q| \le 1$,

$$R(q) = q^{1/5} \prod_{n=0}^{\infty} \frac{(1-q^{5n+1})(1-q^{5n+4})}{(1-q^{5n+2})(1-q^{5n+3})} = \cfrac{q^{1/5}}{1+\cfrac{q}{1+\cfrac{q^2}{1+\cfrac{q^3}{1+\ddots}}}}, \qquad (9.29)$$

Then $R(1) = \varphi - 1$, where φ is our old friend the golden ratio, see Exercise 2.31, and $R(q)$ may be thought of as a q-analogue of the golden mean.

Ramanujan showed that $R(e^{-\pi\sqrt{r}})$ is algebraic for each rational number r; Sloane's sequence A082682 in [156] gives the exact values of $r_n = R(e^{-\pi\sqrt{n}})$

for $1 \leq n \leq 10$. In particular, famously,

$$r_2 = \sqrt{\frac{5+\sqrt{5}}{2}} - \frac{1+\sqrt{5}}{2}.$$

We highly recommend to our readers that they browse through Berndt's edition of Ramanujan's notebooks [13] and the Andrews–Berndt edition of Ramanujan's 'lost notebook' [5] (see also [6]), since just listing Ramanujan's contributions to this particular subject deserves a separate volume.

Turning to the end of Section 9.4, a recent unifying presentation on the more general Seidel–Stern theorem and its relatives, where terms may be complex, is to be found in [12]. The basic building blocks are as follows, where Z_n represents the nth partial quotient.

Theorem 9.31 (The Seidel–Stern theorem, 1846) *If each a_n is positive then the sequences Z_{2n} and Z_{2n+1} are monotonic and convergent. If, in addition, $\sum_n a_n$ diverges then Z_n converges.*

Theorem 9.32 (The Stern–Stolz theorem, 1860) *If Z_n converges then $\sum_n |a_n|$ diverges.*

Theorem 9.33 (Van Vleck's theorem, 1901) *Suppose that $0 \leq \theta < \pi/2$ and that $|\arg(b_n)| \leq \theta$ whenever $a_n \neq 0$. Then the sequences Z_{2n} and Z_{2n+1} converge. Further, Z_n converges if and only if $\sum_n |a_n|$ diverges.*

Examples and pictures in [29, 30], and elsewhere, show the need for such restrictions to rule out period-3 and higher-period behaviour of the convergents. They are based on the irregular fraction $\mathcal{S}(b)$ given by

$$\mathcal{S}(b) = \cfrac{1^2 b_1^2}{1 + \cfrac{2^2 b_2^2}{1 + \cfrac{3^2 b_3^2}{1 + \ddots}}} \tag{9.30}$$

where the string (b_n) is periodic and is most interesting when all terms have the same modulus. The case of period 2 is the setting for Ramanujan's AGM fraction. It is convenient to set (9.30) obeys $t_n = q_{n-1}/n!$, where p_n/q_n is the nth partial convergent of $\mathcal{S}(b)$, so that

$$t_n = \frac{1}{n}\, t_{n-1} + \frac{n-1}{n}\, b_{n-1}^2 t_{n-2}. \tag{9.31}$$

For example, with b_n of period 3 we obtain Figure 9.2 for

$$(b_1, b_2, b_3) = (\exp(i\pi/4), \exp(i\pi/4), \exp(i\pi/4 + 1/\sqrt{2})). \tag{9.32}$$

Note the scaling is that suggested by (9.28).

Exercise 9.34 (Pictures for $\mathcal{R}$) In the original Ramanujan fraction setting, draw graphs with $|b_1| = b_2| = 1$ corresponding to that of Figure 9.2. You should see three cases depending on whether none, one or two of the parameters are roots of unity. However, in all cases the graphs produce points lying on two circles and look nothing like Figure 9.2.

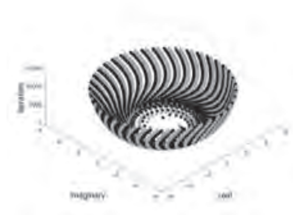

Figure 9.2 Dynamics for cycles of length 3. Shown are the iterates $\sqrt{n}t_n$ for t_n given by (9.31) with the choice (9.32). The odd iterates are light and the even iterates are dark.

We remark that the 'magic' appearance of the identities (9.20) and (9.25) is not accidental: the explicit form of the functions $S_n(t)$ and $\tilde{S}_n(t)$ is the output of the so-called *algorithm of creative telescoping* due to Gosper and Zeilberger, which can be found in [126]. The algorithm is implemented in some computer algebra systems, including Maple and Mathematica.

It is interesting to note that recurrence equations like (9.22) and (9.26) encode a lot of number theory in addition to the material explored above. In recent years such *Apéry-like* difference equations and their generalisations have become a subject of independent interest [4, 171].

While the irrationality proof for $\zeta(2)$ prefigures that for $\zeta(3)$, the most direct proof of the irrationality of π is probably Ivan Niven's 1947 short proof [120]. It illustrates well the ingredients of many more difficult proofs of the irrationality of other constants and indeed of Lindemann's proof of the transcendence of π, which builds on on Hermite's 1873 proof of the transcendence of e.

Theorem 9.35 ([120]) *The number π is irrational.*

Proof Let $\pi = a/b$, the quotient of positive integers. We define the polynomials $f(x) = x^n(a - bx)^n/n!$ and

$$F(x) = f(x) - f^{(2)}(x) + f^{(4)}(x) - \cdots + (-1)^n f^{(2n)}(x);$$

the positive integer n will be specified later. Since $n!f(x)$ has integral coefficients and terms in x of degree not less than n, the polynomial $f(x)$ and its derivatives $f^{(j)}(x)$ have integral values for $x = 0$; also for $x = \pi = a/b$, since $f(x) = f(a/b - x)$. By elementary calculus we have

$$\frac{\mathrm{d}}{\mathrm{d}x}(F'(x)\sin x - F(x)\cos x) = F''(x)\sin x + F(x)\sin x = f(x)\sin x$$

and

$$\int_0^\pi f(x)\sin x\,\mathrm{d}x = \big(F'(x)\sin x - F(x)\cos x\big)\Big|_0^\pi = F(\pi) + F(0). \quad (9.33)$$

Now $F(\pi) + F(0)$ is an *integer*, since $f^{(j)}(0)$ and $f^{(j)}(\pi)$ are integers. But, for $0 < x < \pi$,

$$0 < f(x)\sin x < \frac{\pi^n a^n}{n!},$$

so that the integral in (9.33) is positive but less than 1 for sufficiently large n. Thus (9.33) is false, and so is our assumption that π is rational. □

This proof can be enhanced to cover $\zeta(2)$ as Niven did later [121].

There is a deep connection between the (classical) orthogonal polynomials with respect to a linear functional $\mathcal{L}\colon \mathbb{C}[x] \to \mathbb{C}$ and the continued fraction expansions of the generating function $\sum_{n=0}^{\infty} \mathcal{L}(x^n) z^n$ for its moments; this has nontrivial applications to the evaluation of Kronecker–Hankel determinants. We refer the interested reader to the highly accessible review [89] of this story (see also [50, pp. 91–99]).