

Crouching AGM, Hidden Modularity

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To Mourad Ismail, with warm wishes from three continents

ABSTRACT. Special arithmetic series $f(x) = \sum_{n=0}^{\infty} c_n x^n$, whose coefficients c_n are normally given as certain binomial sums, satisfy ‘self-replicating’ functional identities. For example, the equation

$$\frac{1}{(1+4z)^2} f\left(\frac{z}{(1+4z)^3}\right) = \frac{1}{(1+2z)^2} f\left(\frac{z^2}{(1+2z)^3}\right)$$

generates a modular form $f(x)$ of weight 2 and level 7, when a related modular parametrization $x = x(\tau)$ is properly chosen. In this note we investigate the potential of describing modular forms by such self-replicating equations as well as applications of the equations that do not make use of the modularity. In particular, we outline a new recipe of generating AGM-type algorithms for computing π and other related constants. Finally, we indicate some possibilities to extend the functional equations to a two-variable setting.

1. INTRODUCTION

Modular forms and functions form a unique enterprise in the world of special functions. They are innocent looking q -series, at the same time highly structured and possess numerous links to other parts of mathematics. In our exposition below we will try to hide the modularity of objects under consideration as much as possible, just pointing out related references to the literature where the modular origin is discussed in detail.

One way of thinking of modular forms is through Picard–Fuchs linear differential equations [25, Section 5.4]. The concept can be illustrated on the example

$$f_7(x) = \sum_{n=0}^{\infty} u_n x^n, \tag{1}$$

with coefficients

$$u_n = \sum_{k=0}^n \binom{n}{k}^2 \binom{n+k}{n} \binom{2k}{n} = \sum_{k=0}^n (-1)^{n-k} \binom{3n+1}{n-k} \binom{n+k}{n}^3. \tag{2}$$

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The function $f_7(x)$ represents a level 7 and weight 2 modular form e.g., [10, 29] (see also Section 3 below), and satisfies a linear differential equation, which we record in the form of a recurrence relation for the coefficients

$$(n+1)^3 u_{n+1} = (2n+1)(13n^2 + 13n + 4)u_n + 3n(3n-1)(3n+1)u_{n-1} \quad (3)$$

where $n = 0, 1, 2, \dots$. The single initial condition $u_0 = 1$ is used to start the sequence. This is sequence A183204 in the *OEIS* [23]. Recursions such as (3) are famously known as Apéry-like recurrence equations [2, 10, 26]. The series defining $f_7(x)$ converges in the disc $|x| < 1/27$ as $x = 1/27$ is a singular point of the underlying linear differential equation produced by the recursion.

In this note we will investigate another point of view on the modularity, using functional equations of a different nature. The function $f(x) = f_7(x)$ defined above will be our principal example, while the special functional equation it satisfies will be [12, Theorem 4.4]

$$\frac{1}{(1+4z)^2} f\left(\frac{z}{(1+4z)^3}\right) = \frac{1}{(1+2z)^2} f\left(\frac{z^2}{(1+2z)^3}\right), \quad (4)$$

valid in a suitable neighbourhood of $z = 0$. Note that this equation, together with the initial condition $f(0) = 1$, uniquely determines the coefficients in the Taylor series expansion $f(x) = \sum_{n=0}^{\infty} u_n x^n$. In Section 2 we will address this fact and discuss some variations of Equation (4). In particular, we observe that, in arithmetically interesting instances — those with connections to modular forms — the corresponding sequences appear to satisfy (and possibly are characterized by) strong divisibility properties. Without pretending to fully cover the topic of such functional equations, we list several instances for other modular forms in Section 3 together with some details of the underlying true modular forms and functions. An important feature of this way of thinking of modular forms is applications. One such application — to establishing Ramanujan-type formulas for $1/\pi$ — has already received attention in the literature, e.g., see [13, 15, 28, 29]. In Section 4 we give some related examples for $f_7(x)$ and equation (4), though concentrating mostly on another application of the special functional equations — to AGM-type algorithms. Such algorithms for computing π were first discovered independently by R. Brent [6] and E. Salamin [21] in 1976 (see also [3]). A heavy use of the modularity made later, faster versions by other authors somehow sophisticated. Our exposition in Section 4 follows the ideas in [14] and streamlines the production of AGM-type iterations by freeing them from the modularity argument.

Three-term recurrence relations, which are more general than the one given in (3), naturally appear in connection with orthogonal polynomials [16] — one of the topics mastered by Mourad Ismail. The polynomials have long-existing ties with arithmetic, and the recent work [9, 20, 24, 29] indicates some remarkable links between generating functions of classical Legendre polynomials and arithmetic hypergeometric functions. Interestingly enough, these links allow one to produce a two-variable functional equation that may be thought of as a generalization of (4). This is the subject of Section 5.

2. SELF-REPLICATION VS MODULARITY

The first natural question to ask is how sensitive the dependence of $f(x)$ on the parameters of equation (4) is. In other words, what can be said about a solution $f(x) = f(\lambda, \mu; x) = \sum_{n=0}^{\infty} c_n x^n$, with $c_0 = 1$, to the equation

$$\frac{1}{(1 + \mu z)^2} f\left(\frac{z}{(1 + \mu z)^3}\right) = \frac{1}{(1 + \lambda z)^2} f\left(\frac{z^2}{(1 + \lambda z)^3}\right) \quad (5)$$

when λ and μ are integers? Writing the equation as

$$\sum_{n=0}^{\infty} \frac{c_n z^n}{(1 + \mu z)^{3n+2}} = \sum_{n=0}^{\infty} \frac{c_n z^{2n}}{(1 + \lambda z)^{3n+2}}$$

and applying the binomial theorem to expand both sides into a power series in z , we obtain the recursion

$$c_n = \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n+k+1}{3k+1} (-\lambda)^{n-2k} c_k - \sum_{k=0}^{n-1} \binom{n+2k+1}{3k+1} (-\mu)^{n-k} c_k, \quad (6)$$

for $n = 1, 2, \dots$, which together with $c_0 = 1$ determines the sequence $c_n = c_n(\lambda, \mu)$. Clearly, $c_n(\lambda, \mu) \in \mathbb{Z}$ whenever $\lambda, \mu \in \mathbb{Z}$. Also, the recursion (6) implies that the functional equation (5) completely recovers the analytic solution $f(x)$. The latter fact allows us to think of (4) and, more generally, of (5) as *self-replicating* equations that define the series and function $f(x)$. In spite of the property $c_n \in \mathbb{Z}$ it remains unclear whether these sequences have some arithmetic significance in general. In the sequel, we will refer to instances as *arithmetic* if the generating function $f(x)$ is of modular origin.

The fact that the sequences arising from self-replicating equations such as (4) are integral is useful since this integrality is rather inaccessible from associated differential equations or recurrences such as (3). (It remains an open problem to classify all integer solutions to recurrences of the shape (3), though it is conjectured that the known Apéry-like sequences form a complete list). For Apéry-like sequences, the integrality usually follows from binomial sum representations such as (2). Integrality can be also be deduced by exhibiting a modular parametrization of the differential equation; however, we do not know *a priori* whether such a parametrization should exist [26].

In the arithmetic instances of modular origin, the sequence c_n necessarily satisfies a linear differential equation [25]. On the other hand, for any sequence produced by self-replication, we can (try to) guess a linear differential equation for its generating function by computing a few initial terms. Once guessed, we can then use closure properties of holonomic functions to prove that the solution to the differential equation does indeed satisfy the self-replicating functional equation. If the generating function satisfies a linear differential equation then this somewhat brute experimental approach is guaranteed to find this equation and prove its correctness in finite time. Showing that the sequence is not holonomic is more painful, as the time required by this brute force approach is infinite.

On the other hand, all known arithmetic instances lead to sequences which satisfy strong divisibility properties. For instance, for primes p , these sequences $c(n)$ satisfy the *Lucas congruences*

$$c(n) \equiv c(n_0)c(n_1) \cdots c(n_r) \pmod{p}, \quad (7)$$

where $n = n_0 + n_1p + \cdots + n_rp^r$ is the expansion of n in base p . In the case of Apéry-like numbers, these congruences were shown in [18] and further general results were recently obtained in [1]. In addition, these sequences satisfy, or are conjectured to satisfy, the $p^{\ell r}$ -congruences

$$c(mp^r) \equiv c(mp^{r-1}) \pmod{p^{\ell r}} \quad (8)$$

with $\ell \in \{1, 2, 3\}$, which in interesting cases hold for $\ell > 1$ and are referred to as *supercongruences*, e.g., see [19] and the references therein.

In the following examples, we therefore consider self-replicating functional equations of basic shapes, and search for values of the involved parameters such that the corresponding sequences satisfy such congruences. In each case, in which we observe the Lucas congruences and p^r -congruences, we are able to identify these sequences and relate them to modular forms.

The recursion (6) together with the original self-replicating equation (4) suggest that the choice $\lambda^2 = \mu$ in (5) is of special arithmetic significance. This is substantiated in the next example.

Example 1. We consider the functional relation (5) with integer parameters λ and μ . The terms $c_n(\lambda, \mu)$ of the corresponding sequence are polynomials in λ and μ . The first few are

$$1, \quad 2(\mu - \lambda), \quad 7\mu^3 - 10\lambda\mu + 3\lambda^2 + 2\mu - 2\lambda, \quad \dots$$

Using these initial terms we then determine congruence conditions on the parameters λ, μ , which need to be satisfied in order that the p^r -congruences (8), with $\ell = 1$, hold for all primes p . In the case $\lambda = \mu$ we have $c_n(\lambda, \lambda) = 0$ for $n \geq 1$, and so we assume $\lambda \neq \mu$ in the sequel. Remarkably, the empirical data suggests that these congruences only hold in a finite number of cases, all of modular origin, as well as an infinite family of unclear origin. Specifically, the p^r -congruences appear to hold modulo p^r for all primes p only in the cases $\lambda^2 = \mu$ with

$$\lambda \in \{-2, -1, 2, 4, 16\}$$

and the infinite family of cases $\lambda = -2\mu$ where μ is any even integer. If there exist further cases, then $\min\{|\mu|, |\lambda|\} > 10,000$ (and $|\lambda| > 100,000$ in the particularly relevant case $\lambda^2 = \mu$).

Here is the analysis of the cases when $\lambda^2 = \mu$:

- The case $\lambda = 2$ is the level 7 sequence from the introduction (and Section 3 below).
- The case $\lambda = -2$ is the level 3 sequence $c_n = c_n(-2, 4)$ with

$$\sum_{n=0}^{\infty} c_n z^n = \left(\sum_{n=0}^{\infty} \binom{2n}{n} \binom{3n}{n} z^n \right)^2$$

(see Example 3).

- The case $\lambda = -1$ produces the sequence $c_n(-1, 1) = 2^n \binom{2n}{n}$, which clearly satisfies p^r -congruences (but does not satisfy p^{2r} -congruences). The corresponding generating function $\sum_{n=0}^{\infty} c_n z^n$ is algebraic.
- The case $\lambda = 4$ produces the sequence $c_n = c_n(4, 16)$ with

$$\sum_{n=0}^{\infty} c_n z^n = \left(\sum_{n=0}^{\infty} \binom{2n}{n}^2 \binom{3n}{n} z^n \right)^2,$$

which appears to satisfy p^{3r} -supercongruences. The corresponding modular form has level 3 and weight 4.

- The case $\lambda = 16$ produces the sequence $c_n = c_n(16, 256)$ with (note the exponent)

$$\sum_{n=0}^{\infty} c_n z^n = \left(\sum_{n=0}^{\infty} \binom{2n}{n} \binom{3n}{n} \binom{6n}{3n} z^n \right)^4,$$

which appears to satisfy p^{2r} -supercongruences. The modular form has level 1 and weight 8.

Apparently, the sequences corresponding to $(\lambda, \mu) = (-4\alpha, 2\alpha)$, that is,

$$\frac{1}{(1 + 2\alpha z)^2} f\left(\frac{z}{(1 + 2\alpha z)^3}\right) = \frac{1}{(1 - 4\alpha z)^2} f\left(\frac{z^2}{(1 - 4\alpha z)^3}\right),$$

satisfy p^r congruences for all integers α but do not appear to be holonomic. However, these sequences fail to satisfy Lucas congruences (except modulo 2 and 3, for trivial reasons). In the case $\alpha = 1$ the first few terms of the sequence $c_n = c_n(-4, 2)$ are

$$1, 12, 168, 2496, 38328, 600672, 9539808, 152891520, \dots$$

The first 250 terms do not reveal a linear recurrence with polynomial coefficients, suggesting that the sequence is not holonomic, and we were unable to otherwise identify the sequence. It does take the slightly simplified form

$$c_n = \sum_{k=0}^n d_k d_{n-k}, \quad \text{where } d_n = 1, 6, 66, 852, 11874, 172860, 2586108, \dots$$

Similar comments apply to the case $\alpha = -1$, which results in an alternating sequence. \square

There are many natural shapes of self-replicating functional equations that one could similarly analyze. Here, we restrict ourselves to a variation of (5).

Example 2. In the spirit of the previous example, consider the functional relations

$$\frac{1}{1 + \mu z} f\left(\frac{z}{(1 + \mu z)^2}\right) = \frac{1}{1 + \lambda z} f\left(\frac{z^2}{(1 + \lambda z)^2}\right).$$

We find supercongruences modulo p^{3r} , that is (8) with $\ell = 3$, in the cases $(\lambda, \mu) = (-2, 0)$, $(\lambda, \mu) = (0, -2)$ and $(\lambda, \mu) = (0, 4)$, which correspond to the sequences $\binom{2n}{n}$, $(-1)^n \binom{2n}{n}$ and $\binom{2n}{n}^2$, respectively.

The case $(\lambda, \mu) = (-8, 16)$ produces the sequence a_n with

$$\sum_{n=0}^{\infty} a_n z^n = \left(\sum_{n=0}^{\infty} \binom{2n}{n} \binom{4n}{2n} z^n \right)^2,$$

which appears to satisfy p^{2r} -supercongruences; this is a modular form of level 2 given in Example 3 below.

The cases $(\lambda, \mu) = (-2, 0)$ and $(\lambda, \mu) = (0, -2)$ generalize to the case $(\lambda, \mu) = (-\alpha - 2, \alpha)$, which corresponds to the sequence $(\alpha + 1)^n \binom{2n}{n}$. For obvious reasons we have p^r -congruences for all of these, as well as Lucas congruences and recurrences.

In the cases $(\lambda, \mu) = (2\alpha, 0)$, we appear to have p^r -congruences but no Lucas congruences and no recurrences.

We did not find additional instances of congruences modulo p^r . If there exist any, then $\min\{|\mu|, |\lambda|\} > 10,000$. \square

The arithmetic sequences observed in this section all satisfy strong congruences. It would be interesting to understand to which degree such congruences characterize these arithmetic instances of the self-replication process.

3. SELF-REPLICATING FUNCTIONAL EQUATIONS

For levels $\ell \in \{2, 3, 4, 5, 7\}$ we use the modular functions

$$z_\ell(\tau) = q \left(\prod_{j=1}^{\infty} \frac{1 - q^{\ell j}}{1 - q^j} \right)^{24/(\ell-1)}, \quad \text{where } q = e^{2\pi i \tau},$$

and the corresponding weight two modular forms

$$P_\ell(\tau) = q \frac{d}{dq} \log z_\ell$$

to define implicitly the analytic functions $f_\ell(x)$ by

$$P_2(\tau) = f_2 \left(\frac{z_2(\tau)}{1 + 64z_2(\tau)} \right), \quad P_3(\tau) = f_3 \left(\frac{z_3(\tau)}{1 + 27z_3(\tau)} \right), \quad P_4(\tau) = f_4 \left(\frac{z_4(\tau)}{1 + 16z_4(\tau)} \right),$$

$$P_5(\tau) = f_5 \left(\frac{z_5(\tau)}{1 + 22z_5(\tau) + 125z_5(\tau)^2} \right) \quad \text{and} \quad P_7(\tau) = f_7 \left(\frac{z_7(\tau)}{1 + 13z_7(\tau) + 49z_7(\tau)^2} \right).$$

Explicitly we have

$$f_2(x) = \left(\sum_{n=0}^{\infty} \binom{2n}{n} \binom{4n}{2n} x^n \right)^2 = {}_2F_1 \left(\frac{1}{4}, \frac{3}{4} \middle| 64x \right)^2,$$

$$f_3(x) = \left(\sum_{n=0}^{\infty} \binom{2n}{n} \binom{3n}{n} x^n \right)^2 = {}_2F_1 \left(\frac{1}{3}, \frac{2}{3} \middle| 27x \right)^2,$$

$$f_4(x) = \left(\sum_{n=0}^{\infty} \binom{2n}{n}^2 x^n \right)^2 = {}_2F_1 \left(\frac{1}{2}, \frac{1}{2} \middle| 16x \right)^2,$$

where the standard hypergeometric notation is used, and also

$$f_5(x) = \sum_{n=0}^{\infty} \left\{ \binom{2n}{n} \sum_{k=0}^n \binom{n}{k}^2 \binom{n+k}{k} \right\} x^n,$$

while binomial expressions for the coefficients of $f_7(x)$ are given in (2).

Example 3. Each of these can be characterized by a self-replicating functional equation:

$$\begin{aligned} \frac{1}{1+16z} f_2\left(\frac{z}{(1+16z)^2}\right) &= \frac{1}{1-8z} f_2\left(\frac{z^2}{(1-8z)^2}\right), \\ \frac{1}{(1+4z)^2} f_3\left(\frac{z}{(1+4z)^3}\right) &= \frac{1}{(1-2z)^2} f_3\left(\frac{z^2}{(1-2z)^3}\right), \\ \frac{1}{(1+4z)^2} f_4\left(\frac{z}{(1+4z)^2}\right) &= f_4(z^2), \\ \frac{1}{1+8z} f_5\left(\frac{z}{(1+4z)(1+8z)^2}\right) &= \frac{1}{1+2z} f_5\left(\frac{z^2}{(1+4z)(1+2z)^2}\right), \\ \frac{1}{(1+4z)^2} f_7\left(\frac{z}{(1+4z)^3}\right) &= \frac{1}{(1+2z)^2} f_7\left(\frac{z^2}{(1+2z)^3}\right). \end{aligned}$$

The equations for f_3 and f_7 are discussed in Example 1, and the one for f_2 shows up in Example 2. These instances demonstrate that the example (4) for level 7 may be viewed as part of a bigger family.

We expect similar self-replicating equations for levels 9, 13 and 25; see [11, Section 8]. \square

In order to give some more weight 2 examples, define

$$\begin{aligned} \hat{f}_2(x) &= \sum_{n=0}^{\infty} \binom{2n}{n}^2 \binom{4n}{2n} x^n = {}_3F_2\left(\frac{1}{4}, \frac{1}{2}, \frac{3}{4} \mid 256x\right), \\ \hat{f}_3(x) &= \sum_{n=0}^{\infty} \binom{2n}{n}^2 \binom{3n}{n} x^n = {}_3F_2\left(\frac{1}{3}, \frac{1}{2}, \frac{2}{3} \mid 108x\right), \\ \hat{f}_4(x) &= \sum_{n=0}^{\infty} \binom{2n}{n}^3 x^n = {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \mid 64x\right) \end{aligned}$$

and

$$\hat{f}_5(x) = \sum_{n=0}^{\infty} \left\{ \sum_{k=0}^n (-1)^{n-k} \binom{n}{k}^3 \binom{4n-5k}{3n} \right\} x^n.$$

Example 4. A functional equation for \hat{f}_2 is given by

$$\frac{1}{1+27z} \hat{f}_2\left(\frac{z}{(1+27z)^4}\right) = \frac{1}{1+3z} \hat{f}_2\left(\frac{z^3}{(1+3z)^4}\right).$$

This may be regarded as a cubic version of the functional equations studied in Examples 1 and 2.

A functional equation for \hat{f}_3 is given by the case $\lambda = 4$ in Example 1.

Functional equations for \hat{f}_4 and \hat{f}_5 are of a different type:

$$\begin{aligned} \frac{1}{1+8z} \hat{f}_4 \left(z \left(\frac{1-z}{1+8z} \right)^3 \right) &= \hat{f}_4 \left(z^3 \left(\frac{1-z}{1+8z} \right) \right), \\ \frac{1}{(1+4z)^2} \hat{f}_4 \left(z \left(\frac{1-z}{1+4z} \right)^5 \right) &= \hat{f}_4 \left(z^5 \left(\frac{1-z}{1+4z} \right) \right), \\ \frac{1}{1-5z} \hat{f}_5 \left(z \left(\frac{1-z}{1-5z} \right)^2 \right) &= \hat{f}_5 \left(z^2 \left(\frac{1-z}{1-5z} \right) \right). \quad \square \end{aligned}$$

Example 4 suggests considering functional equations of the type

$$t(z) f(r(z) s^n(z)) = f(r^n(z) s(z))$$

where $r(z)$, $s(z)$ and $t(z)$ are rational functions with

$$r(z) = z + O(z^2), \quad s(z) = 1 + O(z), \quad t(z) = 1 + O(z),$$

and $n \geq 2$ is an integer.

Example 5. We list three more instances that may be compared with the functional equation for f_4 in Example 3:

$$\begin{aligned} g_b(z^2) &= \frac{1}{1+3z} g_b \left(z \frac{1-z}{1+3z} \right), \\ g_c(z^3) &= \frac{1}{1+2z+4z^2} g_c \left(z \frac{1-z+z^2}{1+2z+4z^2} \right) \end{aligned}$$

and

$$g_5(z^5) = \frac{1}{1+3z+4z^2+2z^3+z^4} g_5 \left(z \frac{1-2z+4z^2-3z^3+z^4}{1+3z+4z^2+2z^3+z^4} \right).$$

The solutions to these functional equations that satisfy the initial condition $g(0) = 1$ are given by

$$g_b(x) = \sum_{n=0}^{\infty} \left\{ \sum_{k=0}^{\infty} \binom{n}{k}^2 \binom{2k}{k} \right\} x^n, \quad g_c(x) = \sum_{n=0}^{\infty} \left\{ \sum_{k=0}^{\infty} \binom{n}{k}^3 \right\} x^n$$

and

$$g_5(x) = \sum_{n=0}^{\infty} \left\{ \sum_{k=0}^{\infty} \binom{n}{k}^2 \binom{n+k}{k} \right\} x^n.$$

The functions g_b and g_c may be parameterized by level 6 modular forms, while g_5 may be parameterized by level 5 modular forms, e.g., see [8, Theorem 3.4 and Tables 1 and 2]. The functions g_b , g_c and g_5 are denoted by (c), (a) and (b), respectively, in [2, Eq. (28)]. They are generating functions for the sequences C, A and D, respectively, in [26]. \square

4. FORMULAS FOR $1/\pi$ AND AGM-TYPE ITERATIONS

Example 6. We can use the transformation (4) as $z \rightarrow (1/8)^-$, so that $z/(1+4z)^3 \rightarrow (1/27)^-$ and $z/(1+4z)^3 \rightarrow 1/125$. Applying the asymptotics and techniques from [15, Example 5] we obtain the formula

$$\sum_{n=0}^{\infty} u_n(4+21n) \times \frac{1}{5^{3n+3}} = \frac{1}{8\pi}. \quad (9)$$

This can also be obtained using modular forms, e.g., see [10, Eq. (37) and Table 1].

Consider the limiting case $h \rightarrow h_0^+$, where $h_0 = -(5 + \sqrt{21})/2$, of the transformation [7, Lemmas 4.1 and 4.3]

$$\begin{aligned} & \frac{1}{\sqrt{1+13h+49h^2}} \sum_{n=0}^{\infty} u_n \left(\frac{h}{1+13h+49h^2} \right)^n \\ &= \frac{1}{\sqrt{1+5h+h^2}} {}_3F_2 \left(\begin{matrix} \frac{1}{6}, \frac{1}{2}, \frac{5}{6} \\ 1, 1 \end{matrix} \middle| \frac{1728h^7}{(1+13h+49h^2)(1+5h+h^2)^3} \right), \end{aligned}$$

so that the argument of the ${}_3F_2$ series on the right-hand side tends to $-\infty$, and follow [15, Theorem 2 and Example 2] to obtain

$$\sum_{n=0}^{\infty} u_n \left(\frac{3\sqrt{21}-14}{56} \right)^n = \left(\frac{128(\sqrt{7}-\sqrt{3})}{49(5-\sqrt{21})^2} \right)^{1/3} \frac{\sqrt{\pi}}{3\Gamma(\frac{5}{6})^3} \quad (10)$$

and

$$\sum_{n=0}^{\infty} u_n (6\sqrt{21}-20+15(\sqrt{21}-2)n) \left(\frac{3\sqrt{21}-14}{56} \right)^n = \frac{8\sqrt{7}}{\pi}. \quad (11)$$

The series (11) corresponds to the case $N = 21$ of the identity (39) in [10]. \square

A principal feature of an AGM-type algorithm is a sequence of algebraic approximations a_k , where $k = 0, 1, 2, \dots$, that converge to a given number ξ at a certain rate $r > 1$, so that $|\xi - a_{k+1}| < C|\xi - a_k|^r$ for some absolute constant $C > 0$. If $r = 2$, as for the classical AGM algorithm of Brent [6] and Salamin [21], then it is said to be a quadratic iteration. The next example uses a functional equation to produce quadratic AGM-type iterations to numbers ξ of the form

$$\sum_{n=0}^{\infty} u_n (a_0 + b_0 n) x_0^n = \xi, \quad (12)$$

where a_0, b_0 and x_0 are fixed real algebraic numbers, where the sequence u_n is given in (2). The iterations are based on the self-replicating equation (4).

Example 7. Let a_0, b_0 and x_0 be chosen in accordance with (12), while z_0 is the real solution to

$$\frac{z}{(1+4z)^3} = x_0$$

of the smallest absolute value. Define the sequences a_k , b_k and z_k for all $k \geq 1$ recursively as follows:

$$\begin{aligned} a_{k+1} &= a_k \frac{(1+4z_k)^2}{(1+2z_k)^2} + b_k \frac{4z_k(1+4z_k)^2}{(1+2z_k)^3(1-8z_k)}, \\ b_{k+1} &= 2b_k \frac{(1+4z_k)^3(1-z_k)}{(1+2z_k)^3(1-8z_k)}, \\ z_{k+1} &= \frac{2z_k^2}{1+6z_k+(1+2z_k)\sqrt{1+8z_k}}. \end{aligned}$$

Then a_k converges to ξ in (12) quadratically.

To justify the above iteration, we couple the self-replicating equation (4) with the one obtained from it by differentiation:

$$\begin{aligned} \sum_{n=0}^{\infty} u_n \left(\left(A - \frac{8Bz}{1+4z} \right) + nB \left(1 - \frac{12z}{1+4z} \right) \right) \frac{z^k}{(1+4z)^{3k+2}} \\ = \sum_{n=0}^{\infty} u_n \left(\left(A - \frac{4Bz}{1+2z} \right) + nB \left(2 - \frac{6z}{1+2z} \right) \right) \frac{z^{2k}}{(1+2z)^{3k+2}}. \end{aligned} \quad (13)$$

In addition to the above three sequences we also consider

$$x_k = \frac{z_k}{(1+4z_k)^3}; \quad (14)$$

note that the definition of z_{k+1} implies that

$$x_{k+1} = \frac{z_{k+1}}{(1+4z_{k+1})^3} = \frac{z_k^2}{(1+2z_k)^3}.$$

Then induction on k then shows that

$$\sum_{n=0}^{\infty} u_n (a_k + b_k n) x_k^n = \xi. \quad (15)$$

Indeed, on the k -th step we first define the numbers A , B and $z = z_k$ such that

$$\frac{z}{(1+4z)^3} = x_k, \quad \frac{B}{(1+4z)^2} \left(1 - \frac{12z}{1+4z} \right) = b_k, \quad \frac{1}{(1+4z)^2} \left(A - \frac{8Bz}{1+4z} \right) = a_k$$

and assign to the data

$$x_{k+1} = \frac{z^2}{(1+2z)^3}, \quad b_{k+1} = \frac{B}{(1+2z)^2} \left(2 - \frac{6z}{1+2z} \right) \quad (16)$$

and

$$a_{k+1} = \frac{1}{(1+2z)^2} \left(A - \frac{4Bz}{1+2z} \right). \quad (17)$$

Application of (13) implies the validity of (15) for k replaced with $k+1$; taking $z = z_k$ and eliminating A, B lead to the formulas for a_{k+1} , b_{k+1} and x_{k+1} by means of a_k , b_k and z_k only.

In this construction for x_k sufficiently close to 0 we have $x_{k+1} \approx z_k^2 \approx x_k^2$, so that x_k tends to 0 quadratically. Performing the limit in (15) as $k \rightarrow \infty$ we obtain

$$\xi = \lim_{k \rightarrow \infty} \sum_{n=0}^{\infty} u_n (a_k + b_k n) x_k^n = \lim_{k \rightarrow \infty} a_k.$$

Furthermore, $|\xi - a_k|$ is roughly of magnitude x_k , so that a_k converges to ξ quadratically.

To execute the algorithm one can use (9) to produce the initial conditions

$$a_0 = \frac{4}{125}, \quad b_0 = \frac{21}{125}, \quad x_0 = \frac{1}{125}, \quad z_0 = \left(\frac{\sqrt{2} - 1}{2} \right)^3 = 0.00888347\dots \quad (18)$$

Then for the iteration scheme given by (16) and (17) we have

$$\lim_{n \rightarrow \infty} a_n = \frac{1}{2\pi}$$

and the convergence is quadratic.

Moreover, the formula (10) leads to the initial conditions

$$a_0 = 3 \left(\frac{128(\sqrt{7} - \sqrt{3})}{49(5 - \sqrt{21})^2} \right)^{-1/3}, \quad b_0 = 0, \quad x_0 = \frac{3\sqrt{21} - 14}{56},$$

while z_0 is a real solution of the equation $x_0(1 + 4z)^3 - z = 0$, for which the iteration scheme given by (16) and (17) has the property that

$$\lim_{n \rightarrow \infty} a_n = \frac{\pi^{1/2}}{\Gamma(5/6)^3} = \frac{\Gamma(1/6)^3}{8\pi^{5/2}}$$

with quadratic convergence. In a similar way, the identity (11) leads to a different set of initial conditions such the the iteration scheme given by (16) and (17) generates another sequence that converges to $1/(2\pi)$. \square

Our next example makes use of the identities from Example 4 to produce an iteration scheme that converges quintically to $1/\pi$.

Example 8. Define sequences a_k , b_k , x_k and z_k as follows. Let

$$a_0 = \frac{1}{4}, \quad b_0 = 1, \quad x_0 = -\frac{1}{64}.$$

Recursively, let z_k be the real solution to

$$z^{1/5} \frac{1 - z}{1 + 4z} = x_k^{1/5}$$

that is closest to the origin, and then let

$$a_{k+1} = a_k (1 + 4z_k)^2 + 8b_k \frac{z_k(1 - z_k)(1 + 4z_k)^2}{1 - 22z_k - 4z_k^2},$$

$$b_{k+1} = 5b_k (1 + 4z_k)^2 \frac{1 + 2z_k - 4z_k^2}{1 - 22z_k - 4z_k^2}$$

and

$$x_{k+1} = z_k^5 \frac{1 - z_k}{1 + 4z_k}.$$

Then

$$\lim_{k \rightarrow \infty} a_k = \frac{1}{2\pi}$$

and the rate of convergence is of order 5.

To justify the above algorithm, we differentiate the last formula of Example 4 to get

$$\begin{aligned} \sum_{n=0}^{\infty} \binom{2n}{n}^3 \left(\left(A - \frac{8Bx}{1+4x} \right) + Bn \frac{1-22x-4x^2}{(1-x)(1+4x)} \right) \frac{x^n(1-5x)^{5n}}{(1+4x)^{5n+2}} \\ = \sum_{n=0}^{\infty} \binom{2n}{n}^3 \left(A + 5Bn \frac{1+2x-4x^2}{(1-x)(1+4x)} \right) \frac{x^{5n}(1-x)^n}{(1+4x)^n}. \end{aligned}$$

Consider an iteration scheme that goes as follows. Suppose x_k , a_k and b_k are given, for some k . Compute z , B and A from the formulas

$$z \left(\frac{1-z}{1+4z} \right)^5 = x_k, \quad B \frac{1-22x-4x^2}{(1+4x)^3(1-x)} = b_k$$

and

$$\frac{1}{(1+4x)^2} \left(A - \frac{8Bx}{1+4x} \right) = a_k.$$

Then, let x_{k+1} , b_{k+1} and a_{k+1} be defined by

$$x_{k+1} = \frac{x^5(1-x)}{(1+4x)}, \quad b_{k+1} = \frac{5B(1+2z-4z^2)}{(1-z)(1+4z)}, \quad a_{k+1} = A.$$

These iterations are equivalent to the ones stated in the theorem.

To get initial conditions, consider Bauer's series [8, Table 6, $N = 2$], [27]

$$\sum_{n=0}^{\infty} \binom{2n}{n}^3 \left(\frac{1}{4} + n \right) \left(-\frac{1}{64} \right)^n = \frac{1}{2\pi}.$$

This gives $a_0 = 1/4$, $b_0 = 1$ and $x_0 = -1/64$, as well as the limit

$$\lim_{n \rightarrow \infty} a_n = \frac{1}{2\pi}.$$

The data

$$\begin{aligned} \left| a_0 - \frac{1}{2\pi} \right| &\approx 9.08 \times 10^{-2}, & \left| a_1 - \frac{1}{2\pi} \right| &\approx 6.65 \times 10^{-9}, \\ \left| a_2 - \frac{1}{2\pi} \right| &\approx 8.25 \times 10^{-47}, & \left| a_3 - \frac{1}{2\pi} \right| &\approx 4.57 \times 10^{-239} \end{aligned}$$

is good supporting evidence.

One can also use the series [8, Table 6, $N = 3$]

$$\sum_{n=0}^{\infty} \binom{2n}{n}^3 \left(\frac{1}{6} + n\right) \left(\frac{1}{256}\right)^n = \frac{2}{3\pi}$$

to produce initial conditions $a_0 = 1/6$, $b_0 = 1$, $x_0 = 1/256$ and limiting value

$$\lim_{n \rightarrow \infty} a_n = \frac{2}{3\pi}.$$

Another option is to use the series [8, Table 6, $N = 7$]

$$\sum_{n=0}^{\infty} \binom{2n}{n}^3 \left(\frac{5}{42} + n\right) \left(\frac{1}{4096}\right)^n = \frac{8}{21\pi},$$

to give $a_0 = 5/42$, $b_0 = 1$, $x_0 = 1/4096$ and the limit

$$\lim_{n \rightarrow \infty} a_n = \frac{8}{21\pi}.$$

These have all been tested numerically. There is no practical advantage to starting with different initial conditions, as the speed of convergence is determined by the quintic nature of the algorithm. \square

Observe that the sequence b_k in Example 7 with initial conditions given by (18) has the property

$$\frac{b_k}{b_0} = 2^k \times \sqrt{\frac{1 - 26x_k - 27x_k^2}{1 - 26x_0 - 27x_0^2}}$$

where x_k is given by (14). And, for the sequences b_k in Example 8 we have

$$\frac{b_k}{b_0} = 5^k \times \sqrt{\frac{1 - 64x_k}{1 - 64x_0}}.$$

The factors 2^k and 5^k reflect the quadratic and quintic rates of convergence of the respective iterations, and the factors $1 - 26x - 27x^2$ and $1 - 64x$ are the leading coefficients in the respective differential equations for the functions $f(x)$, e.g., see [10, p. 176].

5. SELF-REPLICATION OF LEGENDRE POLYNOMIALS

Several generating functions of the Legendre polynomials

$$P_n(x) = {}_2F_1\left(-n, n+1 \mid \frac{1-x}{2} \mid 1\right) = \frac{1}{2^n} \sum_{k=0}^n \binom{n}{k}^2 (x-1)^k (x+1)^{n-k}$$

are known but the one we are going to treat in this section is given by

$$F(x; z) = \sum_{n=0}^{\infty} \binom{2n}{n}^2 P_n(x) z^n.$$

The Bailey–Brafman identity [9] allows us to recast the two-variable function as a product of two hypergeometric functions,

$$F\left(\frac{U+V-2UV}{U-V}; \frac{U-V}{16}\right) = {}_2F_1\left(\frac{1}{2}, \frac{1}{2} \middle| U\right) \cdot {}_2F_1\left(\frac{1}{2}, \frac{1}{2} \middle| V\right),$$

and with the help of the quadratic transformation

$${}_2F_1\left(\frac{1}{2}, \frac{1}{2} \middle| u^2\right) = \frac{1}{1+u} \cdot {}_2F_1\left(\frac{1}{2}, \frac{1}{2} \middle| \frac{4u}{(1+u)^2}\right)$$

(essentially, the equation for f_4 in Example 3) we get the following self-replicating identity:

$$\begin{aligned} F\left(\frac{u^2+v^2-2u^2v^2}{u^2-v^2}; \frac{u^2-v^2}{16}\right) \\ = \frac{1}{(1+u)(1+v)} F\left(\frac{(1+uv)(u+v)-4uv}{(1-uv)(u-v)}; \frac{(1-uv)(u-v)}{4(1+u)^2(1+v)^2}\right). \end{aligned} \quad (19)$$

Because of the way the two parameters u and v are tangled in the relation (19), it is not easy to perform an analysis of the equation analogous to the one we have had for (4). Notice, however, that $F(x; z)$ is a particular case of Appell’s F_4 function and that there is a similar-looking identity [17] for Appell’s F_1 function (see also [22, Chap. 4]). As the latter identity is known to be linked to a three-term generalization of the arithmetic-geometric mean, we believe that (19) and the like equations may find some interesting number-theoretic applications.

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