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APPROXIMATING π WITH RAMANUJAN'S MODULAR EQUATIONS

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ABSTRACT. Ramanujan, in Chapter 19 of his Second Notebook gives a number of remarkable quintic and septic modular equations for the eta and related multipliers. Two are of particular interest because they are given in explicit solvable form. This allows us to derive explicit quintic and septic algorithms for pi. The quintic algorithm is especially attractive and its genesis is discussed in some detail.

1. Introduction. There is a close and beautiful relationship between the transformation theory of elliptic integrals and the efficient high precision approximation of pi. The three most recent record calculations are due to Bailey [1] (29.3 million digits in 1986) and to Kanada (33.5 million digits in 1986 and 133.5 million digits in early 1987). Each of these employed the following quartically converging iteration as one of the two algorithms used in the calculation. (It is now customary to declare a record only after a computation has been corroborated by a second calculation using a different algorithm - in these cases related quadratically converging iterations.)

Algorithm 1. Let $\alpha_0 := 6 - 4\sqrt{2}$ and $y_0 := \sqrt{2} - 1$. Let

(a) $y_{n+1} := (1 - \sqrt{1 - y_n^4}) / (1 + \sqrt{1 - y_n^4})$ and let

(b) $\alpha_{n+1} := (1 + y_{n+1})^4 \alpha_n - 2^{2n+3} y_{n+1} (1 + y_{n+1} + y_{n+1}^2)$.

Then

$$0 < \alpha_n - \pi^{-1} < 16 \cdot 4^n e^{-2 \cdot 4^n \pi}.$$

Thirteen iterations suffice for Bailey's and Kanada's calculations. The algorithm is derived and discussed in [4].

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The penultimate record of 17.5 million digits due to Gosper in 1985 used Ramanujan's [7, 8] rapidly converging series

$$\frac{1}{\pi} = \frac{2\sqrt{2}}{9801} \sum_{n=0}^{\infty} \frac{(4n)!}{4^{4n}(n!)^4} [1103 + 26390n] \left(\frac{1}{994}\right)^n.$$

(Each term adds roughly 8 digits.) Like many of Ramanujan's results this appears without proof, the only derivation we know of is in [4].

Algorithm 1 rests on an underlying quartic transformation of the complete elliptic integrals E and K . Ramanujan's series requires computing a 58th degree singular value and so is related to a 58th order transformation. Such transformations (or their associated modular relations) factor into their prime components, a fourth order transformation is just two successive second order transformations. Transformations associated with distinct primes are thus the most interesting. The basic quadratic transformation is the Gaussian arithmetic-geometric mean iteration. Its explicit role in the computation of π was explored in the 70's by Salamin [9] and by Brent [5], its role in the computation of elliptic integrals goes back to Gauss, Lagrange and Legendre. Cubic versions are discussed in [3] and [4]. The most attractive rest on cubic modular identities of Ramanujan.

Currently we wish to explore a particularly attractive fifth order algorithm, for π based on a surprisingly simple fifth order modular identity, also due to Ramanujan. Some parts of this theory appear in [4].

2. A solvable quintic algorithm for π . The following algorithm converges quintically to π .

Algorithm 2. Let $s_0 := s(r)$ and $\alpha_0 := \alpha(r)$. (For $r = 1$, $s_0 = 5(\sqrt{5} - 2)$ and $\alpha_0 = 1/2$.) Let

(a) $s_{n+1} := 25/(z + x/z + 1)^2 s_n$, where $x := 5/s_n - 1$, $y := (x-1)^2 + 7$ and $z := ((x/2)(y + \sqrt{y^2 - 4x^3}))^{1/5}$;

(b) $\alpha_{n+1} := s_n^2 \alpha_n - \sqrt{r} 5^n \left\{ (s_n^2 - 5)/2 + \sqrt{s_n(s_n^2 - 2s_n + 5)} \right\}$.

Then

$$\frac{1}{\alpha_n} \rightarrow \pi \text{ quintically}$$

and, for $r5^n \geq 1$,

$$0 < \alpha_n - \frac{1}{\pi} < 16.5^n \sqrt{r} e^{-5^n \sqrt{r} \pi}.$$

(In fact, $\alpha_n - \pi^{-1} \sim 8\sqrt{r}5^n e^{-5^n \sqrt{r} \pi}$).

For $r = 1$, the first few approximations to π , $\alpha_0^{-1}, \alpha_1^{-1}, \alpha_2^{-1}$ and α_3^{-1} , give 0, 5, 31 and 166 digit agreement respectively. The eleventh approximation agrees through in excess of 66 million digits. The algorithm is quite stable, the intermediate value s_n converges to 1 quintically. The roots involved are always positive. The quantity $\delta := z + x/z$ is a positive root of $\delta^5 - 5x\delta^3 + 5x^2\delta - xy$, with x and y as in the algorithm.

The preceding algorithm rests on the analysis of two functions M_5 and α where, in the notation of the algorithm,

$$s_n := M_5(r5^{2n}) \text{ and } \alpha_n := \alpha(r5^{2n}).$$

The function M_5 is the *quintic multiplier* and iteration (a) is based on Ramanujan's form of the quintic modular equation for M_5 . This is the subject of the next section.

The function α , its role in approximating π and its relation to M_5 will be examined in §4.

3. Ramanujan's quintic modular equation. The *theta function* θ_3 is defined by

$$\theta_3(q) := \sum_{n=-\infty}^{\infty} q^{n^2}.$$

The p^{th} *order multiplier* $\mathcal{M}_p(q)$ is defined by

$$\mathcal{M}_p(q) := \theta_3^2(p^q) / \theta_3^2(q).$$

Two useful ancillary quantities are

$$M_5(n) := \mathcal{M}_5(e^{-\pi\sqrt{n}})$$

and

$$m_n := m_n(r) := 5M_5(r5^{2n}).$$

Ramanujan's quintic modular equation in solvable form (Entry 12 (iii) of Ramanujan's Second Notebook, see [2]) in slightly rewritten form is the following result.

THEOREM 1.

$$\frac{5\theta_3(q^{25})}{\theta_3(q)} = 1 + r_1^{1/5} + r_2^{1/5}$$

where, for $i = 1$ or 2 ,

$$r_i := \frac{1}{2}x(y \pm \sqrt{y^2 - 4x^3})$$

and

$$x := \frac{5\theta_3^2(q^5)}{\theta_3^2(q)} - 1 \quad \text{and} \quad y := (x - 1)^2 + 7.$$

This provides an explicit solvable expression for $\mathcal{M}_5(q^5)$ in terms of $\mathcal{M}_5(q)$. It also provides an explicit solvable expression for $\theta_3(q^{25})$ in terms of $\theta_3(q^5)$ and $\theta_3(q)$. (Some of this is further discussed in the last section.) In terms of m_n this can be written as

$$m_{n+1} = (1 + r_1^{1/5} + r_2^{1/5})^2 / m_n,$$

where

$$x := m_n - 1 \quad \text{and} \quad y \quad \text{and} \quad r_i \quad \text{are as above.}$$

The derivation of (a) of Algorithm 2 is now effected by setting $s_n := 5/m_n$ and $z := r_1^{1/5}$. We observe that $r_1 r_2 = x^5$ so $r_2^{1/5} = x/z$ and only one fifth root need be extracted. The starting value s_0 is computed from the evaluation

$$M_5(1) = \frac{1}{5(\sqrt{5} - 2)}$$

(see [4]).

4. The function α . We need the following standard notations. The *complete elliptic integrals* K and E are defined by

$$K(k) := \int_0^{\pi/2} \frac{dt}{\sqrt{1 - k^2 \sin^2 t}} \quad \text{and} \quad E(k) := \int_0^{\pi/2} \sqrt{1 - k^2 \sin^2 t} dt$$

The *complementary modulus* is $k' := \sqrt{1 - k^2}$. The *complementary integrals* are defined by

$$K'(k) := K(k') \quad \text{and} \quad E'(k) := E(k').$$

These quantities satisfy *Legendre's relation*

$$E(k)K'(k) + E'(k)K(k) - K(k)K'(k) = \pi/2$$

which is pivotal in relating these quantities to π . (All of this is accessible in [12]).

The relationship between theta functions and the elliptic integrals requires introducing two additional theta functions

$$\theta_2(q) := \sum_{n=-\infty}^{\infty} q^{(n+1/2)^2}$$

and

$$\theta_4(q) := \theta_3(-q) = \sum_{n=-\infty}^{\infty} (-q)^{n^2}.$$

Then, for $|q| < 1$,

$$K(k) = \frac{\pi}{2} \theta_3^2(q),$$

where

$$k(q) := k = \frac{\theta_2^2(q)}{\theta_3^2(q)}, \quad k' = \frac{\theta_4^2(q)}{\theta_3^2(q)}$$

and

$$q = e^{-\pi K'(k)/K(k)}.$$

The p^{th} order multiplier is then

$$\mathcal{M}_p(l, k) := \frac{K(k)}{K(\ell)} = \mathcal{M}_p(q),$$

where $l = k(q)$ and $k := k(q^p)$.

We now define α by

$$\alpha(r) := \frac{E'(k)}{K(k)} - \frac{\pi}{4K^2(k)} \quad k := k(e^{-\pi\sqrt{r}}).$$

One can then deduce, from Legendre's relation, that

$$\frac{\pi}{4} = K[\sqrt{r}E - (\sqrt{r} - \alpha(r))K]$$

which may be viewed as a one sided Legendre relation. For r rational, both $\alpha(r)$ and $k(r)$ are algebraic. Since K/π and E/π are both easily computed at algebraic values (quadratically by the AGM, with p^{th} order convergence by related modular transformations) we see the first connection with approximation to pi.

We can write down a theta function expansion for α , namely

$$\alpha(r) := \frac{[\pi^{-1} - \sqrt{r}4q\dot{\theta}_4(q)/\theta_4(q)]}{\theta_3^4(q)},$$

where $\dot{\theta}_4(q) := \frac{d\theta_4(q)}{dq}$ and $q := e^{-\pi\sqrt{r}}$. From this it is easily deduced that $\alpha(r) \rightarrow 1/\pi$ as $r \rightarrow \infty$ and that

$$\alpha(r) - \frac{1}{\pi} \sim 8\left(\sqrt{r} - \frac{1}{\pi}\right)e^{-\pi\sqrt{r}}.$$

It is thus of interest to iteratively calculate α at large values of r . The key to this calculation is the next theorem, a proof of which is in [4].

THEOREM 2. *Let p and r be positive. Let $l := k(q)$ and $k = k(q^p)$. Then*

$$\alpha(p^2r) = \frac{\alpha(r)}{\mathcal{M}_p^2(l, k)} - \sqrt{r} \left\{ \frac{l^2}{\mathcal{M}_p^2(l, k)} - pk^2 + \frac{pk^{12}k}{\mathcal{M}_p(l, k)} \frac{d\mathcal{M}_p(l, k)}{dk} \right\}.$$

This, for $p := 5$, specializes to the following.

THEOREM 3. *If r is positive and $s(r) := M_5^{-1}(r)$, then*

$$\alpha(25r) = s^2(r)\alpha(r) - \sqrt{r} \left\{ \frac{s^2(r) - 5}{2} + \sqrt{s(r)(s^2(r) - 2s(r) + 5)} \right\}.$$

This is proved by using the explicit form of the quintic multiplier given by Ramanujan (Entries 13 and 14 of his second notebook) and a fair bit of careful algebraic manipulation. The hardest part is getting the correct formula to prove. The reader is spared the details. The iteration of the above formula for α provides (b) of Algorithm 2. The starting value requires knowing that $\alpha(1) = 1/2$. For the calculation of $\alpha(r)$ and $s(r)$ at various simple rational r one should see [4] and [11]. This is closely connected to the calculation of singular values for the modular function λ and except for a very few numbers is difficult

5. Some generalities. For p an odd prime the quantities $v(q) := (k(q))^{1/4}$ and $u(q) := (k(q^p))^{1/4}$ satisfy an irreducible equation of degree $p + 1$ in the variables u and v . This is the *p th order modular equation*, $\Omega_p(v, u)$. For example,

$$\Omega_3(v, u) = u^4 - v^4 + 2uv(1 - u^2v^2)$$

and

$$\Omega_5(v, u) = u^6 - v^6 + 5u^2v^2(u^2 - v^2) + 4uv(1 - u^4v^4).$$

The multiplier $\mathcal{M}_p(l, k)$ is rational in u and v . One can base a p^{th} order algorithm for π on Theorem 2 and iterative solution of the p^{th} order modular equation, and indeed this is the basis for Algorithms 1 and 2. The problem is that, for $p \geq 5$, the Galois group of Ω_p over $\mathbf{Q}_p(u)$ is a non-solvable group of order $p(p^2 - 1)$. Here \mathbf{Q}_p denotes \mathbf{Q} adjoin the p^{th} roots and the 8^{th} roots of unity).

From Theorem 1 and the identities

$$\begin{aligned} k &:= \theta_2^2/\theta_3^2, & k' &= \theta_4^2/\theta_3^2, \\ \theta_4^2 + \theta_2^2 &= \theta_3^2, & \theta_4(q) &= \theta_3(-q) \end{aligned}$$

we easily deduce that $u(q^5)$ is solvable over $\mathbf{Q}_p(u(q), u(q^{1/5}))$, while as above, $u(q^5)$ is not solvable over $\mathbf{Q}_p(u(q))$. What is happening is the following. Both $u(q^p) := (-1)^{(p^2-1)/8}(k(q^{p^2}))^{1/4}$ and $u(q^{1/p}) := (k(q))^{1/4}$ are roots of $\Omega_p(\cdot, u(q)) = 0$. Also, $u(q^{1/p})$ is of degree $p+1$ over $\mathbf{Q}_p(u)$. And so the Galois group of Ω_p over $\mathbf{Q}_p(u(q), u(q^{1/5}))$ is of order dividing $p(p-1)$, which, obviously, for $p = 5, 7, 11$ and 13 (and in fact in general), is solvable. Thus, one is guaranteed solvable p^{th} order algorithms of all prime order. (See [6, 10, 11]).

Ramanujan gives solvable fifth and seventh order modular identities for the *eta multipliers*

$$N_5(q) := \eta^2(q)/\eta^2(q^{1/5})$$

and

$$N_7(q) := \eta^2(q)/\eta^2(q^{1/7}),$$

where the *eta function* is defined by

$$\eta(q) := q^{1/12} \prod_{n=1}^{\infty} (1 - q^{2n}).$$

(These are in Entries 12 and 18 of Chapter 19 of his Second Notebook). The seventh order form, slightly recast, is given below.

THEOREM 4.

$$7N_7(q^7) = (u^{1/7} + v^{1/7} + w^{1/7} - 1)^2 / (7N_7(q))$$

where u, v and w are the roots of

$$x^3 - ax^2 - bx + 1 = 0,$$

where

$$a := 57 + 14(7N_7(q))^2 + (7N_7(q))^4$$

and

$$b := 289 + 126(7N_7(q))^2 + 19(7N_7(q))^4 + (7N_7(q))^6.$$

This allows for the explicit construction of a solvable septic algorithm for π - though not as cleanly as in the quintic case.

There are two additional pieces one needs. First is the septic update for α

$$\alpha(49r) = s^2(r)\alpha(r) - \sqrt{r} \left\{ \frac{s^2(r) - 7}{2} + s(r)4t(1-t) \right\}$$

where $t^4 := kl$ and

$$s(r) := \mathcal{M}_7^{-1}(l, k) := \mathcal{M}_7^{-1}(e^{-\pi\sqrt{r}}).$$

Second is a solvable relation between M_7 and N_7 , namely

$$(49\mathcal{M}_7^2 - 1)N_7^3 - 8\mathcal{M}_7^2N_7^2 + 8\mathcal{M}_7^2N_7 + \mathcal{M}_7(\mathcal{M}_7^2 - 1) = 0.$$

Also one can show that

$$4t(1-t) = \frac{7\mathcal{M}_7 + \mathcal{M}_7^{-1}}{7N_7 + N_7^{-1}},$$

and therefore only \mathcal{M}_7 and N_7 need enter the iteration.

To the best of our knowledge no one is in possession of an explicit solvable form of an endecadic (11th order) modular equation. Determining it, and the concomitant endecadic algorithm for π presents an interesting computational problem. Even in the 5th and 7th order case the proofs of Ramanujan's modular identities, due to Berndt [2], are facilitated by the symbolic computation package MACSYMA.

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