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CUBIC AND HIGHER ORDER ALGORITHMS FOR π

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ABSTRACT. We show that the theory of elliptic integral transformations may be employed to construct iterative approximations for π of order p (p any prime). Details are provided for two, three and seven. The cubic case proves amenable to surprisingly complete analysis.

0. **Introduction.** Simple three term recursion relations based on the arithmetic-geometric mean iteration of Gauss and Legendre have recently been used to compute in excess of 4 million digits of π. (See [10].) These algorithms, first suggested by Brent [4] and Salamin [9], converge quadratically and arise from quadratic transformations of elliptic integrals. (See also [1], [2], [3] and [7].) Iterations that converge faster than quadratically can be based on higher order elliptic transformations. As we shall see, the cubic transformation and its concommitant cubically converging algorithm for π is particularly amenable to analysis. In general, for any prime p, we will show that it is possible to construct an algorithm for pi that converges in such a manner that the error at the nth step is like the pth power of the error at the preceding step.

1. **Preliminaries.** We first summarize the pieces of the theory of elliptic integrals that we require. This information is all pleasantly accessible in Cayley [5]. The *complete elliptic integral of the first kind of modulus* k is defined by

$$K := K(k) := \int_0^1 \frac{dx}{\sqrt{[(1-x^2)(1-k^2x^2)]}}. \tag{1-1}$$

The *complete elliptic integral of the second kind* is defined by

$$E := E(k) := \int_0^1 \frac{\sqrt{(1-k^2x^2)}}{\sqrt{(1-x^2)}}\,dx. \tag{1-2}$$

The *conjugate modulus* k' is defined by $k' := \sqrt{(1-k^2)}$. It is elementary that

$$\frac{dK}{dk} = \frac{E}{k(k')^2} - \frac{K}{k}. \tag{1-3}$$

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Legendre's relation between elliptic integrals of the first and the second kind is

$$EK' + E'K - KK' = \frac{\pi}{2} \tag{1-4}$$

where $K' := K(k')$ and $E' := E(k')$. This elementary, though not entirely straightforward, formula is at the heart of the algorithm for π because it allows the calculation of π to be related to the tractable problem of calculating elliptic integrals. In fact, we shall see that K/π is straightforward to calculate iteratively. From (1-3) E/π may also be computed and from (1-4) π may be extracted rationally. (One can always compute derivatives of these analytic limits by differentiating iteratively.)

If p is an odd prime it transpires that there exists a unique polynomial of degree $p+1$ in u and v called the *modular equation* of degree p (which we shall denote by $m_p(u, v)$) and a rational function of degree p in u and v called the *multiplier* and denoted by $M_p := M_p(u, v)$ so that

$$M_p K(\lambda) = K(k), \qquad 0 < k < \lambda < 1. \tag{1-5}$$

provided $u := k^{1/4}$ and $v := \lambda^{1/4}$ satisfy

$$m_p(u, v) = 0. \tag{1-6}$$

The modular equation has real integral coefficients and has coefficients of u^{p+1} and v^{p+1} of absolute value 1. The modular equation and the multiplier are related by

$$pM_p^2 = \frac{\lambda(\lambda')^2}{k(k')^2}\frac{dk}{d\lambda}. \tag{1-7}$$

Note that if m_p is known then $dk/d\lambda$ may be easily computed and, hence, M_p as well.

2. **General algorithms for complete elliptic integrals, π and log.** For fixed p let

$$v_0 := \lambda^{1/4} \in (0, 1)$$

and define v_i recursively by demanding that $v_{i+1} \in (0, v_i)$ satisfies

$$m_p(v_{i+1}, v_i) = 0. \tag{2-1}$$

This uniquely determines v_{i+1} (see [6]). Furthermore, v_i converges to zero and one can show that

$$v_{i+1} \sim 2^{(1-p)/2} v_i^p.$$

Thus, from (1-5), since $K(0) = \pi/2$,

$$\frac{K(\lambda)}{\pi} = \frac{1}{2}\left(\prod_{i=0}^{\infty} \frac{1}{M_p(v_{i+1}, v_i)}\right), \qquad v_0 = \lambda^{1/4}. \tag{2-2}$$

This algebraic product (in λ) for $K(\lambda)/\pi$ exhibits pth-order convergence. In order to generate π, note that from (1–4) with $k := 1/\sqrt{2}$ (so that $K' = K$ and $E' = E$) we have

$$2EK - K^2 = \frac{\pi}{2}$$

or

$$2\left(\frac{E}{\pi}\right)\left(\frac{K}{\pi}\right) - \left(\frac{K}{\pi}\right)^2 = \frac{1}{2\pi}. \tag{2-3}$$

From (2-2) we may calculate K/π with the initial value $v_0 := 2^{-1/8}$ (i.e. $k := 1/\sqrt{2}$) and from (2-2) and (1-3) we may calculate $(1/\pi)(dK/dk)$ and, hence, E/π. The derivative in (1-3) may be computed iteratively from the derivatives of the partial products in (2-2). This whole process converges with pth-order. We shall examine the details for $p = 2$, 3 and 7 later.

Since

$$\left|\log\left(\frac{4}{k}\right) - K(\sqrt{[1-k^2]})\right| = 0(k^2 \log k),$$

and since we may calculate K at the same rate as π, we may use the above methods to generate log as well. (See [3], [4] and [7].) This, of course, gives us an entrée to the computation of all the elementary functions and related constants.

3. **The quadratic case.** The quadratic transformation does not conform to exactly the same rules as the transformations of order an odd prime. One form of the quadratic transformation (see [5]) gives

$$K(k) = (1+\gamma)(K(\gamma))$$

where

$$\gamma := \frac{1-\sqrt{(1-k^2)}}{1+\sqrt{(1-k^2)}} \qquad \text{(modular equation)}$$

or equivalently

$$k = \frac{2\sqrt{\gamma}}{1+\gamma}$$

Whence,

$$K(k) = \frac{\pi}{2}\prod_{n=1}^{\infty}(1+k_n) \qquad k_0 := k$$

where

$$k_{n+1} := \frac{1-\sqrt{(1-k_n^2)}}{1+\sqrt{(1-k_n^2)}}.$$

A little manipulation yields:

$$\frac{2}{\pi}K(k) = \lim \alpha_n$$

where

$$k_{n+1} := \left(\frac{1-\sqrt{(1-k_n^2)}}{k_n}\right)^2, \qquad k_0 := k \tag{3-1}$$

and

$$\alpha_{n+1} := (1+k_{n+1})\alpha_n, \qquad \alpha_0 := 1. \tag{3-2}$$

Upon differentiation we have:

$$\frac{2}{\pi}\frac{dK(k)}{dk} = \lim \beta_n$$

where

$$j_{n+1} := \frac{2k_{n+1}j_n}{k_n\sqrt{(1-k_n^2)}}, \qquad j_0 := 1 \tag{3-3}$$

and

$$\beta_{n+1} := (1+k_{n+1})\beta_n + j_{n+1}\alpha_n, \qquad \beta_0 := 0. \tag{3-4}$$

(Note that $j_n = dk_n/dk$ and $\beta_n = d\alpha_n/dk$.) From the above, (1-3) and (2-3) with the starting value $k := 1/\sqrt{2}$ we deduce that

$$\pi_n := \frac{2\sqrt{2}}{\alpha_n \cdot \beta_n} \to \pi \tag{3-5}$$

and that the convergence is quadratic.

This algorithm for π (equations (3-1), (3-2), (3-3), (3-4) and (3-5)) behaves numerically like those discussed in [1], [2], [4], and [10]. The twentieth iteration, for example, is correct through more than 1.4 million digits.

4. **The cubic case.** The cubic modular equation is

$$u^4 - v^4 - 2u^3v^3 + 2uv = 0. \tag{4-1}$$

The cubic multiplier is given by

$$M_3(u, v) = \frac{v}{v+2u^3}. \tag{4-2}$$

We can use the explicit formula for quartic equations to solve (4-1) for u as a function of v. We have

$$y := \sqrt[3]{[4v^2(1-v^8)]}$$

$$R := \sqrt{(v^6+y)}$$

$$D := \sqrt{\left(2v^6 - y + \frac{4v-2v^9}{R}\right)}$$

and

$$u = \frac{v^3}{2} + \frac{D-R}{2}. \tag{4-3}$$

This value of u is the unique root of (4-1) in $(0, v)$. If we likewise solve (4-1) for v as a function of u we have

$$y = \sqrt[3]{[4u^2(1-u^8)]}$$
$$R = \sqrt{(u^6 + y)}$$
$$D = \sqrt{\left(2u^6 - y + \frac{4u - 2u^9}{R}\right)}$$

and

$$v = -\frac{u^3}{2} + \frac{R+D}{2}. \tag{4-4}$$

This value of v is the unique root in $(u, 1)$. We proceed to generate the sequence of v_i as in Section 2. We discover that by using (4-3) (with $v := v_n$ and $u := v_{n+1}$) and subtracting (4-4) (with $u := v_n$ and $v := v_{n-1}$) we have

$$v_{n+1} = v_n^3 - \sqrt{\{v_n^6 + \sqrt[3]{[4v_n^2(1-v_n^8)]}\}} + v_{n-1}. \tag{4-5}$$

This surprisingly simple solution of the quartic (4-1) can be coupled with the multiplier (4-2) to generate an algorithm for π (see Section 2).

THE CUBIC ALGORITHM. Let

$$v_{n+1} := v_n^3 - \sqrt{\{v_n^6 + \sqrt[3]{[4v_n^2(1-v_n^8)]}\}} + v_{n-1}. \tag{4-6}$$

$$w_{n+1} := \frac{(2v_n^3 + v_{n+1}(3v_{n+1}^2 v_n^2 - 1))}{(2v_{n+1}^3 - v_n(3v_{n+1}^2 v_n^2 - 1))} w_n. \tag{4-7}$$

$$\alpha_{n+1} := \left(\frac{2v_{n+1}^3}{v_n} + 1\right)\alpha_n. \tag{4-8}$$

$$\beta_{n+1} := \left(\frac{2v_{n+1}^3}{v_n} + 1\right)\beta_n + (6w_{n+1}v_n - 2v_{n+1}w_n)\frac{v_{n+1}^2 \alpha_n}{v_n^2} \tag{4-9}$$

where $v_0 := 2^{-1/8}$, $v_1 := 2^{-7/8}((1-3^{1/2})2^{-1/2} + 3^{1/4})$, $w_0 := 1$, $\alpha_0 := 1$ and $\beta_0 := 0$. Then

$$\pi_n := \frac{8 \cdot 2^{1/8}}{\alpha_n \cdot \beta_n} \to \pi \tag{4-10}$$

and the convergence is cubic.

Note that $\alpha_n \to 2K(v_0^4)/\pi$, that $w_n = dv_n/dv_0$ (implicitly differentiating (4-1)) and that $\beta_n = d\alpha_n/dv_0$. The algorithm is now constructed, essentially as in Section 2 or Section 3. The value v_1 is computed from v_0 using (4-3). The

cubic convergence follows directly from (4-1). Note that with $v_n =: v$ and $v_{n+1} =: u$ we have

$$v_{n+1} + \frac{v_{n+1}^4}{2v_n} = \frac{v_n^3}{2} + v_n^2 \cdot v_{n+1}^3$$

whence,

$$v_{n+1} \sim \frac{v_n^3}{2}.$$

The following table illustrates the cubic convergence. The second row of the table is the number of correct digits of π provided by the nth iteration of the algorithm.

n	1	2	3	4	5	6
correct digits	2	10	34	106	327	989

5. **The septic case.** For $p > 3$ the modular equation is of too high a degree to solve explicitly. However, it is quite practical to solve this equation by Newton's method. For the case $p = 7$ the modular equation is given by

$$(1-u^8)(1-v^8) - (1-uv)^8 = 0. \tag{5-1}$$

This equation is tempting to employ in algorithms since it is an eighth degree polynomial which is particularly easy to evaluate. Also since u behaves like $v^7/8$, if we use Newton's method to solve (5-1) we have a very good initial estimate. The multiplier is given by

$$M_7(u, v) = \frac{v(1-uv)(1-uv+u^2v^2)}{v-u^7}. \tag{5-2}$$

In order to calculate π we now follow the steps outlined in section 2, namely:

a] Generate $v_0, v_1, v_2 \cdots$ by inverting the septic modular equation (5.1) starting with $v_0 := 2^{-1/8}$.

b] Generate $w_0, w_1, w_2 \cdots$ where $w_i := dv_i/dv_0$ and $w_0 := 1$. (Note that dv_{i+1}/dv_i can be calculated from (5-1) and a].)

c] Generate $\alpha_0, \alpha_1, \ldots, \alpha_n$ where

$$\alpha_{i+1} := \frac{1}{M_7(v_{i+1}, v_i)}\,\alpha_i$$

and $\alpha_0 := 1$. This converges to $2K(1/\sqrt{2})/\pi$.

d] Generate $\beta_0, \beta_1, \ldots, \beta_n$ where $\beta_i := d\alpha_i/dv_0$ and $\beta_0 := 0$.

e] $\pi_n := (8 \cdot 2^{1/8})/(\alpha_n \cdot \beta_n) \to \pi$.

This process converges septically. The first three iterations yield, respectively 7, 64 and 464 correct digits of π. We note that the only non-rational part of the above algorithm is step a].

6. **Concluding remarks.** The steps a] to e] can be used to construct an algorithm of order p, provided one knows the modular equation of order p. We need only replace the septic modular equation and multiplier by those of pth order. From (1-7) we can calculate the multiplier from the modular equation.

The most time consuming step is a], the solution of the modular equation by Newton's method. It is worth remembering, however, that even with the explicit quadratic and cubic algorithms that square roots and cube roots must be extracted to high precision and that this also utilizes Newton's method. In fact, it appears at least as efficient to solve the cubic modular equations by Newton's method in the cubic algorithms as it is to generate the $\{v_i\}$ from the recursion, which requires extracting both a square and a cube root. The crucial fact about Newton's method is that it is self correcting. Thus, at each step of an inversion, calculations need only be performed to twice the precision of the previous step. This allows one to show that inverting an algebraic equation is of much the same time complexity as a single full precision multiplication (See [3] and [4]). It is thus legitimate to call the septic algorithm "septic" because the root extraction is not governing the order of the approximation. Of course, one can always turn a quadratic algorithm into a quartic algorithm and so on by composing two steps of the iteration. What is interesting is that in our case the algorithms are genuinely of prime order.

Calculating high order modular equations is a tractable though not completely elementary problem. Modular equations up to degree twenty are presented by Cayley in tabular form in [6].

From a complexity point of view all the algorithms for π are roughly equivalent requiring $0(\log nM(n))$ single digit operations to calculate n digits of π ($M(n)$ denotes the number of single digit operations required to multiply two n digit numbers together; a fast multiplication is $0(n \log n \log n)$). For any particular one of these algorithms the update (i.e. steps a] through e] inclusive of the septic case) require a constant number of multiplications, divisions, additions and root extraction and each of these operations is $0(M(n))$. Further details may be found in [3] and [4].

It is possible to show that the iterates are monotone decreasing in the following sense. Let $v_i(p)$ denote the ith iterate of the pth order iteration. Then $v_i(p)$ decreases as p^i increases.

It is also possible to show that the error in the π algorithm behaves like $v_i(p)$. From these considerations one can show that the algorithm based on the modular equation of order 19 produces more than 19^i digits of π on the ith

iteration. In particular, the 7th iteration produces in excess of a billion (U.S.) digits.

Finally, we note that considerable material on elliptic functions and integrals may be found in [11], and that in [8] Ramanujan uses the same ingredients to construct many fascinating explicit approximations to π.

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