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More Quadratically Converging Algorithms for π

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Abstract. We present a quadratically converging algorithm for π based on a formula of Legendre's for complete elliptic integrals of modulus $\sin(\pi/12)$ and the arithmetic-geometric mean iteration of Gauss and Legendre. Precise asymptotics are provided which show this algorithm to be (marginally) the most efficient developed to date. As such it provides a natural computational check for the recent large-scale calculations of π.

1. The Algorithms. The arithmetic-geometric mean of Gauss and Legendre is defined, for $k \in (0,1]$, by

$$a_{n+1} = \frac{a_n + b_n}{2}, \quad b_{n+1} = \sqrt{a_n b_n}, \quad c_{n+1} = \frac{1}{2}(a_n - b_n) \tag{1}$$

with $a_0 := 1$, $b_0 := \sqrt{1-k^2} := k'$, $c_0 := k$. The common limit of $\{a_n\}$ and $\{b_n\}$ we call $\mathrm{AGM}(k')$. The remarkable utility of the above iteration stems from two observations. Firstly,

$$0 < b_n < b_{n+1} < a_{n+1} < a_n \quad \text{and} \quad c_{n+1} = c_n^2/4a_{n+1},$$

which show that both sequences converge quadratically. Secondly, their common limit can be expressed in terms of complete elliptic integrals of the first kind $K := K(k)$, that is,

$$\frac{\pi}{2\,\mathrm{AGM}(k')} = \int_0^{\pi/2} \frac{dt}{\sqrt{1-k^2\sin^2 t}} := K. \tag{2}$$

Complete elliptic integrals of the second kind

$$E := E(k) := \int_0^{\pi/2} \sqrt{1-k^2\sin^2 t}\, dt$$

can also be calculated from the arithmetic-geometric mean iteration. Precisely,

$$(K-E)/K = 1/2\left(c_0^2 + 2c_1^2 + \cdots + 2^n c_n^2 + \cdots\right). \tag{3}$$

This powerful tool for computing elliptic integrals can be used to derive algorithms for π as follows. Let $E' := E(k')$ and $K' := K(k')$. (These are the complete elliptic integrals in the *conjugate modulus* $k' = \sqrt{1-k^2}$.) Then, Legendre's formula relating these quantities is

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

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If we observe that $k = k'$ for $k = 1/\sqrt{2}$, then we can combine (2), (3) and (4) to get

$$\pi = \frac{2\left(\mathrm{AGM}(1/\sqrt{2})\right)^2}{1 - \sum_{j=0}^{\infty} 2^j c_j^2}, \tag{5}$$

which upon truncation provides the desired algorithm. That is, if $k = 1/\sqrt{2}$ and

$$\pi_n := \frac{2(a_{n+1})^2}{1 - \sum_{j=0}^{n} 2^j c_j^2},$$

then π_n converges to π quadratically. In fact,

$$0 < \pi - \pi_n < \frac{\pi^2 2^{n+4} e^{-\pi 2^{n+1}}}{\left(\mathrm{AGM}(1/\sqrt{2})\right)^2}$$

(see [9] or the final section) and

$$\pi - \pi_{n+1} < \frac{2^{-(n+1)}}{\pi^2}(\pi - \pi_n)^2.$$

A continuum of algorithms can be derived from (4) using different values of k. However, most other choices of k double the amount of work and slow the convergence by necessitating the estimation of both $\mathrm{AGM}(k)$ and $\mathrm{AGM}(k')$. Formula (5) is given by Brent [3] and by Salamin [9].

We base our algorithms on two other formulas of Legendre [6, p. 60]. For $k := \sin(\pi/12) = (\sqrt{6} - \sqrt{2})/4$

$$\frac{\pi}{4} = \sqrt{3}K\left(E - \frac{\sqrt{3}+1}{2\sqrt{3}}K\right). \tag{6}$$

For $k := \cos(\pi/12) = (\sqrt{6} + \sqrt{2})/4$

$$\frac{\pi}{4} = \frac{1}{\sqrt{3}}K\left(E - \frac{\sqrt{3}-1}{2\sqrt{3}}K\right). \tag{7}$$

Compare these to (4) with $k = 1/\sqrt{2}$, which collapses to

$$\frac{\pi}{4} = K\left(E - \frac{1}{2}K\right). \tag{8}$$

The two new algorithms which are similarly derived from (6) and (7) on substitution of (2) and (3) are as follows:

ALGORITHM 1. Let

$$a_0 := 1, \quad b_0 := \frac{\sqrt{6}+\sqrt{2}}{4} \quad \text{and} \quad c_0 := \frac{\sqrt{6}-\sqrt{2}}{4}.$$

Let

$$a_{n+1} = \frac{a_n + b_n}{2}, \quad b_{n+1} = \sqrt{a_n b_n} \quad \text{and} \quad c_{n+1} = c_n^2/4a_{n+1}.$$

If

$$\pi_n := \frac{2(a_{n+1})^2}{\left(1 - \sum_{j=0}^{n} 2^j c_j^2\right)\sqrt{3} - 1},$$

then

$$0 \leqslant \pi - \pi_n < \frac{\sqrt{3}\,\pi^2 2^{n+4} e^{-\sqrt{3}\,\pi 2^{n+1}}}{(\mathrm{AGM}(b_0))^2}$$

and

$$\pi - \pi_{n+1} < \frac{\sqrt{3}\,2^{-(n+1)}}{\pi^2}(\pi - \pi_n)^2.$$

ALGORITHM 2. Let

$$a_0 := 1, \quad b_0 := \frac{\sqrt{6} - \sqrt{2}}{4} \quad \text{and} \quad c_0 := \frac{\sqrt{6} + \sqrt{2}}{4}.$$

Let

$$a_{n+1} = \frac{a_n + b_n}{2}, \quad b_{n+1} = \sqrt{a_n b_n} \quad \text{and} \quad c_{n+1} = c_n^2/4a_{n+1}.$$

If

$$\pi_n := \frac{6(a_{n+1})^2}{\left(1 - \sum_{j=0}^{n} 2^j c_j^2\right)\sqrt{3} + 1},$$

then

$$0 \leqslant \pi - \pi_n < \frac{\pi^2 2^{n+4} e^{-\pi 2^{n+1}/\sqrt{3}}}{\sqrt{3}\,(\mathrm{AGM}(b_0))^2}$$

and

$$\pi - \pi_{n+1} < \frac{2^{-(n+1)}}{\sqrt{3}\,\pi^2}(\pi - \pi_n)^2.$$

The upper bounds on the error provided in the algorithms are remarkably sharp. The error analysis will be provided in the next section. We observe that this analysis rederives Salamin's estimate for the error in (5).

ALGORITHM 1

n	0	1	2	3	4	5	6	7	8	9
# Correct digits	1	6	15	34	71	146	298	599	> 1000	> 1000
# Predicted	2*	6	15	34	71	147*	298	600*	1205	2414

ALGORITHM 2

n	0	1	2	3	4	5	6	7	8	9
# Correct digits	0	0	3	9	21	46	94	196	398	800
# Predicted	0	0	3	9	21	46	96*	197*	398	801*

GAUSS - SALAMIN (FORMULA 5)

n	0	1	2	3	4	5	6	7	8	9
# Correct digits	0	2	7	18	40	83	170	344	693	⩾ 1000
# Predicted	0	2	7	18	40	83	170	344	693	1392

The correct digits row of each table was computed using a 1,000 digit scaled integer arithmetic. An entry of k in the prediction row means that the error was $< 10^{-k}$. The predicted values were computed from the error estimates. The entries marked with asterisks, where the bounds exceed the observed accuracies, all result from counting exact digits rather than error. We observe that Algorithm 1 converges considerably faster ($\sqrt{3}$ times as many digits correct) than the Gauss-Salamin estimate. It is, however, marginally more complex, requiring a single additional root extraction at the initialization and a single additional multiplication in the final computation of π_n.

Formula (5) has been employed recently by Tamura and Kanada [10] to compute 4,194,293 digits of π. They checked these results by rerunning the program at twice the precision rather than using an asymmetric version of (4). Perhaps Algorithm 1 would provide a convenient means of verifying such calculations. They have subsequently computed 16,777,216 digits on a HITAC M-280H, using an arctangent relation of Gauss for verification to 10,013,395 digits on a HITAC S-810/20 (private communication).

Other quadratic algorithms for π may be found in [2], [7] and [8]. These are also based on the arithmetic-geometric mean iteration. They are slightly less efficient though they require somewhat less of the theory of elliptic integrals. Formulas (6) and (7) of Legendre may also be found in [11, p. 527] as may all the necessary elliptic function theory. Of course, much of this is readily accessible in the original Gauss [4] and Legendre [6]. The monograph [5] has a wealth of material on computational aspects of the AGM. For a history of the calculation of π see [1], [10] or [12]; and for the relationship between the AGM and the rapid calculation of the elementary functions see [2], [3] or [7].

2. Convergence Rates. Let $q := e^{-\pi K'/K}$ denote the *nome* [11] of the iteration. Then (2) shows that $K'/K = \mathrm{AGM}(k')/\mathrm{AGM}(k)$. We restrict our analysis to $k = \sin(\pi/12)$, $k = \cos(\pi/12)$ and $k = \sin(\pi/4)$. (With minor modifications, this error analysis extends to analogous algorithms based on identities such as (18)–(21).) For these values, as with various other algebraic k, one can solve for K'/K. (One has, respectively, $\sqrt{3}$, $1/\sqrt{3}$ and 1 [11].) When there can be no confusion we shall abbreviate $\mathrm{AGM}(k')$ to AGM. The fundamental result ([2], [5]) is that $(c_n/4a_n)^{1/2^{n-1}}$ increases to q quadratically. Thus,

$$c_n < 4a_n q^{2^{n-1}} \tag{9}$$

and

$$c_n \sim 4\,\mathrm{AGM}\,q^{2^{n-1}}. \tag{10}$$

In each case we have

$$\pi_n = \frac{a_{n+1}^2}{\alpha - K'\left(\sum_{j=0}^{n} 2^{j-1}c_j^2\right)/K}.$$

When $k = \sin(\pi/12)$, then $\alpha = (\sqrt{3} - 1)/2$; when $k = \cos(\pi/12)$, then $\alpha = (\sqrt{3} + 1)/6$; and when $k = \cos(\pi/4)$, then $\alpha = 1/2$.

Let d_n denote the denominator of π_n and let $\beta := K'/K$. Then

$$\pi_{n+1} - \pi_n = \frac{a_{n+2}^2}{d_{n+1}} - \frac{a_{n+1}^2}{d_n} = \frac{a_{n+1}^2 \beta 2^n c_{n+1}^2}{d_{n+1} d_n} - \frac{a_{n+1}^2 - a_{n+2}^2}{d_{n+1}}$$
$$= \left(\beta \frac{\pi_{n+1}\pi_n}{a_{n+2}^2}\right) 2^n c_{n+1}^2 - \pi_{n+1} \frac{(a_{n+1} + a_{n+2})}{a_{n+2}^2} c_{n+2}.$$

Since $4a_{n+2}c_{n+2} = c_{n+1}^2$, one checks that the first term dominates the second and so $\pi_n < \pi_{n+1} < \pi$.

Thus,

$$\pi_{n+1} - \pi_n < \frac{\beta \pi^2 2^n}{(\mathrm{AGM})^2} c_{n+1}^2 \tag{11}$$

and

$$\pi_{n+1} - \pi_n > \frac{\beta \pi_{n+1}^2}{a_{n+2}^2} (2^n - 2^{-1}) c_{n+1}^2. \tag{12}$$

Summing (11), and using $c_{k+1}/4\,\mathrm{AGM} < (c_k/4\,\mathrm{AGM})^2$, produces

$$\pi - \pi_n < \beta \frac{\pi^2}{(\mathrm{AGM})^2} 2^n c_{n+1}^2 \left(1 + (4\mathrm{AGM})^2 \sum_{j=1}^{\infty} 2^j \left(\frac{c_{n+2}}{4\mathrm{AGM}}\right)^{2^j}\right).$$

Since, in each case, $\mathrm{AGM} \geqslant 1/2$, we may bound this last summation by $1 + \sum_{j=1}^{\infty}(2c_{n+2}^2)^j$. This, since $c_2 < 1/2$ in each case, is bounded above by $1 + 4c_{n+2}^2$. Thus

$$\pi - \pi_n < \beta \frac{\pi^2}{(\mathrm{AGM})^2} 2^n c_{n+1}^2 (1 + 4c_{n+2}^2). \tag{13}$$

With (12) this shows that

$$\frac{\beta \pi_{n+1}^2}{a_{n+2}^2}(2^n - 2^{-1}) c_{n+1}^2 < \pi - \pi_n < \frac{\beta \pi^2}{(\mathrm{AGM})^2} 2^{n+1} c_{n+1}^2. \tag{14}$$

Now (9) and (13) show that

$$0 < \pi - \pi_n < \frac{\beta \pi^2}{(\mathrm{AGM})^2} 2^{n+4} e^{-\pi\beta 2^{n+1}}, \tag{15}$$

since $a_{n+1}^2(1 + 4c_{n+2}^2) < 1$. Finally (14) shows that

$$\pi - \pi_{n+1} < \frac{2^{-(n+1)}}{\beta \pi^2} (\pi - \pi_n)^2. \tag{16}$$

Now substitution of the appropriate β produces the error estimates of the three algorithms. The previous considerations can easily be used to show that

$$\pi - \pi_n \sim \frac{K'}{K} \frac{\pi^2}{(\mathrm{AGM})^2} 2^{n+1} c_{n+1}^2$$
$$\sim \frac{K'}{K} \pi^2 2^{n+4} e^{-\pi(K'/K)2^{n+1}}. \tag{17}$$

We finish with a few observations. Firstly, the number of decimal digits (up to rounding) guaranteed by the algorithms is at least the integer part of

$$\pi\left(\frac{K'}{K}\right)2^{n+1}\log_{10}e-(n+4)\log_{10}2-\log_{10}\left(\frac{K'}{K}\frac{\pi^2}{\mathrm{AGM}^2}\right),$$

which for most intents and purposes is well estimated by the first term. Thus, asymptotically our Algorithm 1 gives $\sqrt{3}$ times the digits of Salamin's method and Algorithm 2 gives $1/\sqrt{3}$ times that accuracy. Secondly, addition of Eqs. (6) and (7) produces Legendre's identity (4) with $k := \sin(\pi/12)$ and Salamin's error analysis [9] shows, not surprisingly, that this behaves like Algorithm 2. Indeed, all of the nonsymmetric algorithms in [9] converge more slowly than the symmetric form.

Finally, we observe that a single AGM computation of π essentially relies on being able to express (i) K' in terms of K and (ii) E' in terms of E and K. For $k = \sin(\pi/4)$ obviously $E = E'$ while for $k = \sin(\pi/12)$ (6) and (7) show that $K = \sqrt{3}E - E'$, because $K' = \sqrt{3}K$. Ideally, one would wish to find similar identities to (6) or (7) in which K'/K is larger than $\sqrt{3}$. This is always possible but in general, at the expense of a more complicated initial value. Other examples do, however, exist. With $k := \sqrt{2} - 1 = \tan(\pi/8)$ one has $K' = \sqrt{2}K$. Moreover, $k' = 2\sqrt{k}/(1 + k)$ in this case and one can show that $E' = (1 + k)E - kK'$ (on using the Landen transform ([9, Eq. 4], [5])). This produces

$$E' = \sqrt{2}E - (2 - \sqrt{2})K. \tag{18}$$

Substitution of this formula into (4) produces

$$\frac{\pi}{2} = K(2\sqrt{2}E - 2K) \tag{19}$$

and two more formulas for π (whose rates are given by (17) and are governed by $\sqrt{2}$ and $1/\sqrt{2}$).

There is, in fact, a general class of elliptic integral identities like (6), (7), (8) and (19) whose derivation and application relies on the theory of higher-order elliptic transformations. This will be described in a future paper. For example,

$$\frac{\pi}{2} = K\left(2\sqrt{7}E - (\sqrt{7} + 2)K\right) \tag{20}$$

when $k := \sqrt{2}(3 - \sqrt{7})/8$ and

$$\frac{\pi}{2} = K\left(2\sqrt{9}E - \left(\sqrt{9} + (27)^{1/4}(\sqrt{6} - \sqrt{2})\right)K\right) \tag{21}$$

when $k := (\sqrt{2} - 3^{1/4})(\sqrt{3} - 1)/2$.

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