How to compute 45 million digits of π

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University of Michigan Undergrad Math Club, April 16 2009

An iterative algorithm for π

- Initialize: $x_0 := \sqrt{2}, \quad y_1 := 2^{1/4}, \quad \pi_0 := 2 + \sqrt{2}.$
- Iteration: $x_{n+1} = \dfrac{\sqrt{x_n} + 1/\sqrt{x_n}}{2}$
- Iteration: $y_{n+1} = \dfrac{y_n\sqrt{x_n} + 1/\sqrt{x_n}}{1 + y_n}$
- Iteration: $\pi_n = \pi_{n-1}\dfrac{1 + x_n}{1 + y_n}$

n	$\pi_n - \pi$
0	$2.7262 \cdot 10^{-1}$
1	$1.0141 \cdot 10^{-3}$
2	$7.3762 \cdot 10^{-9}$
3	$1.8313 \cdot 10^{-19}$
4	$5.4721 \cdot 10^{-41}$
5	$2.4061 \cdot 10^{-84}$
6	$2.3085 \cdot 10^{-171}$

Remarks

- Computing square-roots to high accuracy is easy: Newton's method, continued fractions...
- For $n \geq 2$ we have $0 < \pi_n - \pi < 10^{-2^{n+1}}$
- $n = 24$ iterations gives at least 45 million correct digits of π
- By comparison:
  - Archimedes method of inscribed polyhedra produces 1 accurate digit of π after 24 steps.
  - The best known Machin-like arctangent formulae give about 56 correct digits after 24 terms.
  - $56 < 45000000$

In this talk, we will explain (with proof) why the algorithm works.

The AGM

Consider the following recursion (due to Gauss):

- Given: a_0, b_0 real numbers with $0 < b_0 \leq a_0$
- $a_{n+1} := \dfrac{a_n + b_n}{2}$ (arithmetic mean)
- $b_{n+1} := \sqrt{a_n b_n}$ (geometric mean)

By the arithmetic-geometric mean inequality,

$$b_n \leq b_{n+1} \leq a_{n+1} \leq a_n$$

So

$$M(a_0, b_0) := \lim_{n\to\infty} a_n = \lim_{n\to\infty} b_n$$

exists, and is uniquely determined by a_0, b_0.

Elliptic Integrals

For $k \in (0,1)$: The complete elliptic integral of the first kind:

$$K(\alpha) := \int_0^{\pi/2} \frac{d\theta}{\sqrt{1-\alpha^2 \sin^2\theta}}$$

The complete elliptic integral of the second kind:

$$E(\alpha) := \int_0^{\pi/2} \sqrt{1-\alpha^2 \sin^2\theta}$$

Theorem

For any $\alpha \in (0,1)$ with $\beta = \sqrt{1-\alpha^2}$ we have

$$M(1,\alpha) = \frac{\pi}{2K(\beta)}$$

Proof

Let

$$T(a,b) := \frac{2}{\pi}\int_0^{\pi/2} \frac{d\theta}{\sqrt{a^2\cos^2\theta + b^2\sin^2\theta}} = \frac{2}{\pi a}K(\sqrt{1-\frac{b^2}{a^2}})$$

Substituting $t = b\tan\theta$ gives $dt = bd\theta/\cos^2\theta$ and

$$T(a,b) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{dt}{\sqrt{(a^2+t^2)(b^2+t^2)}}.$$

Setting $u = \frac{1}{2}(t - ab/t)$ gives

- $du = \frac{1}{2}(1 + ab/t^2)dt = (\sqrt{u^2+ab})\dfrac{dt}{t}$
- $\dfrac{(a+b)^2}{4} + u^2 = \dfrac{1}{t^2}(a^2+t^2)(b^2+t^2)$ so

$$T(\frac{a+b}{2}, \sqrt{ab}) = T(a,b).$$

Proof (continued)

Thus, $T(a_n, b_n) = T(a_0, b_0)$ for all n.

$$\begin{aligned} T(a_0, b_0) &= T(M(a_0, b_0), M(a_0, b_0)) \\ &= \frac{2}{\pi} \int_0^{\pi/2} \frac{d\theta}{M(a_0, b_0)} \\ &= \frac{1}{M(a_0, b_0)} \\ &= \frac{1}{a_0 M(1, b_0/a_0)} \end{aligned}$$

As

$$T(a_0, b_0) = \frac{2}{\pi a_0} K\left(\sqrt{1 - \frac{b_0^2}{a_0^2}}\right),$$

we are done upon setting $a_0 = 1$, $b_0 = \alpha$, $\beta = \sqrt{1 - \alpha^2}$.

Legendre's Relation

We want to relate special values of K to π. The Key is:

Theorem

For any $\alpha \in (0,1)$ *and* $\beta = \sqrt{1-\alpha^2}$ *we have*

$$K(\alpha)E(\beta) + K(\beta)E(\alpha) - K(\alpha)K(\beta) = \frac{\pi}{2}.$$

Proof (Berndt-Almkvist): Let $a = \alpha^2$, $b = \beta^2 = 1 - \alpha$. We claim

1. $$\frac{d}{da}(E(\alpha) - K(\alpha)) = -\frac{E(\alpha)}{2b}, \qquad \frac{d}{da}E(\alpha) = \frac{E(\alpha) - K(\alpha)}{2a}$$
2. $$\frac{d}{da}(E(\beta) - K(\beta)) = \frac{E(\beta)}{2a}, \qquad \frac{d}{da}E(\beta) = -\frac{E(\beta) - K(\beta)}{2b}$$

Proof of Legendre's Relation (continued)

Granting the identities 1–2, and putting (for the sake of brevity)

$$K := K(\alpha), \quad K' := K(\beta), \qquad E := E(\alpha), \quad E' := E(\beta)$$

we have:

$$\begin{aligned}
&\frac{d}{da}(KE' + K'E - KK') = \frac{d}{da}(EE' - (E-K)(E'-K')) \\
=&\frac{E-K}{2a}E' - E\frac{E'-K'}{2b} + \frac{E}{2b}(E'-K') - (E-K)\frac{E'}{2a} \\
=&0
\end{aligned}$$

so $KE' + K'E - KK' = (E-K)K' + E'K$ is constant. From the definitions as integrals, we easily compute

$$\lim_{\alpha\to 0}\left((E-K)K' + E'K\right) = 0 + 1 \cdot \frac{\pi}{2} = \frac{\pi}{2}.$$

Proof of identities 1–2

The identity 2 follows easily from 1, using $b = 1 - a$. To prove 1:

$$\frac{d}{da}(E-K) = -\frac{d}{da}\int_0^{\pi/2} \frac{a\sin^2\theta}{\sqrt{1-a\sin^2\theta}}d\theta$$

$$= \frac{E}{2a} - \frac{1}{2a}\int_0^{\pi/2} \frac{d\theta}{(1-a\sin^2\theta)^{3/2}}$$

But

$$\frac{d}{d\theta}\frac{\sin\theta\cos\theta}{\sqrt{1-a\sin^2\theta}} = \frac{1}{a}\sqrt{1-a\sin^2\theta} - \frac{b}{a}(1-a\sin^2\theta)^{-3/2}$$

so

$$\frac{d}{da}(E-K) = \frac{E}{2a} - \frac{E}{2ab} + \frac{1}{2b}\int_0^{\pi/2} \frac{d}{d\theta}\frac{\sin\theta\cos\theta}{\sqrt{1-a\sin^2\theta}}$$

$$= \frac{E}{2a}\left(1 - \frac{1}{b}\right) = -\frac{E}{2b}$$

A useful corollary

The second identity in 1 follows easily from definitions.

Corollary

Let $L(\alpha) := \frac{d}{d\alpha}K(\alpha)$. *Then*

$$\pi = \sqrt{2}K(\frac{1}{\sqrt{2}})L(\frac{1}{\sqrt{2}}).$$

To prove this Corollary, we'll need:

Lemma

$$L(\alpha) = \frac{E(\alpha) - \beta^2 K(\alpha)}{\alpha\beta^2}.$$

Proof of the Corollary

Granting the Lemma, we get $E = \alpha\beta^2 L + \beta^2 K$. Hence, writing $L = L(\alpha)$, $L' = L(\beta)$ etc., Legendre's relation gives:

$$\begin{aligned} \frac{\pi}{2} &= K(\beta\alpha^2 L' + \alpha^2 K') + K'(\alpha\beta^2 L + \beta^2 K) - KK' \\ &= \alpha\beta(\alpha K L' + \beta K' L) \end{aligned}$$

Substituting $\alpha = 1/\sqrt{2}$ (so $\beta = \sqrt{1-\alpha^2} = 1/\sqrt{2}$) gives:

$$\pi = \sqrt{2} K(\frac{1}{\sqrt{2}}) L(\frac{1}{\sqrt{2}})$$

as claimed.

Proof of the Lemma

We wish to prove: $\frac{dK}{d\alpha} = \frac{E - \beta^2 K}{\alpha\beta^2} = \frac{E - (1-\alpha^2)K}{\alpha(1-\alpha^2)}$.

By definition, we have

$$K = \int_0^{\pi/2} (1 - \alpha^2 \sin^2\theta)^{-1/2} d\theta$$
$$= \int_0^{\pi/2} \left(1 + \frac{1}{2}\frac{\alpha^2 \sin^2\theta}{1!} + \frac{1\cdot 3}{2^2}\frac{\alpha^4 \sin^4\theta}{2!} + \cdots\right) d\theta$$
$$= \frac{\pi}{2}\left(1 + \left(\frac{1}{2^1\cdot 1!}\right)^2 \alpha^2 + \left(\frac{1\cdot 3}{2^2\cdot 2!}\right)^2 \alpha^4 + \left(\frac{1\cdot 3\cdot 5}{2^3\cdot 3!}\right)^2 \alpha^6 + \cdots\right)$$

Proof of the Lemma (continued)

Similarly,

$$E = \frac{\pi}{2}\left(1 - \left(\frac{1}{2^1 \cdot 1!}\right)^2 \frac{\alpha^2}{1} - \left(\frac{1 \cdot 3}{2^2 \cdot 2!}\right)^2 \frac{\alpha^4}{3} - \left(\frac{1 \cdot 3 \cdot 5}{2^3 \cdot 3!}\right)^2 \frac{\alpha^6}{5} - \cdots\right)$$

Expanding everything in power series, the relation

$$\alpha(1-\alpha^2)\frac{dK}{d\alpha} = E - (1-\alpha^2)K$$

is equivalent to the following combinatorial identity:

$$(2n)^2\left(\frac{1}{2^{2n}}\binom{2n}{n}\right)^2 = (2n-1)^2\left(\frac{1}{2^{2n-2}}\binom{2n-2}{n-1}\right)^2$$

which is obvious.

Relating L and the AGM

Recall that $K(\beta) = \dfrac{\pi}{2M(1,\alpha)}$. Want: similar formula for L

Theorem

Let $a_0 = 1$, $a_0' = 0$ and $b_0 = \alpha$, $b_0' = 1$ and for $n \geq 0$ define

$$a_{n+1} = \frac{a_n + b_n}{2} \qquad b_{n+1} = \sqrt{a_n b_n}$$
$$a'_{n+1} = \frac{a'_n + b'_n}{2} \qquad b'_{n+1} = \frac{a'_n\sqrt{b_n/a_n} + b'_n\sqrt{a_n/b_n}}{2}$$

Setting $M'(a_0, b_0) := \lim_{n\to\infty} a'_n = \lim_{n\to\infty} b'_n$, we have

$$L(\beta) = \frac{\pi}{2}\frac{\beta}{\alpha}\frac{M'(1,\alpha)}{M(1,\alpha)^2}.$$

Proof of the theorem

Differentiating $K(\beta) = \dfrac{\pi}{2M(1,\alpha)}$ with respect to α gives

$$L(\beta)\frac{d\beta}{d\alpha} = -\frac{\pi}{2M(1,\alpha)^2} \cdot \frac{d}{d\alpha}M(1,\alpha)$$

Since $\beta = \sqrt{1-\alpha^2}$, we have $\dfrac{d\beta}{d\alpha} = -\alpha/\beta$ so the proof is complete once we know:

$$M'(1,\alpha) = \frac{d}{d\alpha}M(1,\alpha).$$

But this is clear, as

$$a_n' = \frac{da_n}{d\alpha} \qquad b_n' = \frac{db_n}{d\alpha}$$

for all n by definition.

The formula for π

Combining $\pi = \sqrt{2}K(1/\sqrt{2})L(1/\sqrt{2})$ with our formulae for K, L:

Theorem

Let $a_0 = 1$, $b_0 = 1/\sqrt{2}$, $a'_0 = 0$, $b'_0 = 1$ *and define*

$$a_{n+1} = \frac{a_n + b_n}{2} \qquad b_{n+1} = \sqrt{a_n b_n}$$

$$a'_{n+1} = \frac{a'_n + b'_n}{2} \qquad b'_{n+1} = \frac{a'_n\sqrt{b_n/a_n} + b'_n\sqrt{a_n/b_n}}{2}$$

Then

$$\pi = 2\sqrt{2}\frac{M(1, 1/\sqrt{2})^3}{M'(1, 1/\sqrt{2})} = \lim_{n\to\infty} 2\sqrt{2}\frac{b_{n+1}^2 a_{n+1}}{a'_{n+1}}$$

The x, y-recursion.

Set $x_n := a_n/b_n$ for $n \geq 0$ and $y_n := b'_n/a'_n$ for $n \geq 1$. Put:

$$\pi_n := 2\sqrt{2}\frac{b_{n+1}^2 a_{n+1}}{a'_{n+1}}$$

so $\pi = \lim_n \pi_n$. Note that $x_0 = \sqrt{2}$, $y_1 = 2^{1/4}$, $\pi_0 = 2 + \sqrt{2}$. We have

$$\frac{\pi_n}{\pi_{n-1}} = \frac{(b_{n+1}/b_n)^2(a_{n+1}/a_n)}{(a'_{n+1}/a'_n)} = \frac{1 + x_n}{1 + y_n}.$$

Also,

$$x_{n+1} = \frac{a_{n+1}}{b_{n+1}} = \frac{a_n + b_n}{2\sqrt{a_n b_n}} = \frac{\sqrt{a_n/b_n} + \sqrt{b_n/a_n}}{2} = \frac{\sqrt{x_n} + 1/\sqrt{x_n}}{2}.$$

A similar calculation gives the claimed recursion for y_n.