Jonathan Borwein, Pi and the AGM

Richard P. Brent

Australian National University
and CARMA, University of Newcastle

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Why π?

Why was Jon interested in π?

Perhaps because it is *transcendental* but appears in many mathematical formulas. For example, here are some that I like:

$$\begin{aligned} e^{i\pi} &= -1, && \text{(Euler)},\\ \frac{\pi}{4} &= \arctan(1) = 1 - \tfrac{1}{3} + \tfrac{1}{5} - \cdots && \text{(Gregory/Leibnitz)},\\ &= \arctan(\tfrac{1}{2}) + \arctan(\tfrac{1}{3}) && \text{(Euler)},\\ &= 4\arctan(\tfrac{1}{5}) - \arctan(\tfrac{1}{239}) && \text{(Machin)}. \end{aligned}$$

You can prove arctan formulas using

$$\tan(x+y) = \frac{\tan(x) + \tan(y)}{1 - \tan(x)\tan(y)}\,,$$

e.g. put $x := \arctan(1/2)$, $y := \arctan(1/3)$, then

$$\tan(x+y) = \frac{1/2 + 1/3}{1 - 1/6} = 1 = \tan(\pi/4).$$

Formulas involving π and the Gamma function

The Gamma function

$$\Gamma(z) := \int_0^\infty x^{z-1} e^{-x}\, dx$$

generalises the factorial, as $\Gamma(n+1) = n!$ for $n \in \mathbb{N}$.
The Gamma function has a "reflection formula"

$$\Gamma(1-z)\Gamma(z) = \frac{\pi}{\sin \pi z}$$

and a "duplication formula"

$$\Gamma(z)\Gamma(z+\tfrac{1}{2}) = 2^{1-2z}\pi^{1/2}\Gamma(2z)$$

that involve π. Putting $z = \frac{1}{2}$ in either of these gives

$$\Gamma(\tfrac{1}{2}) = \sqrt{\pi}.$$

π and infinite products

There are infinite products that converge to π. Perhaps the first (historically) is Viète's formula (1593):

$$\frac{2}{\pi} = \frac{\sqrt{2}}{2} \cdot \frac{\sqrt{2+\sqrt{2}}}{2} \cdot \frac{\sqrt{2+\sqrt{2+\sqrt{2}}}}{2} \cdots$$

A different one is by John Wallis (1655):

$$\frac{\pi}{2} = \prod_{n=1}^{\infty} \frac{4n^2}{4n^2-1} = \frac{2}{1} \cdot \frac{2}{3} \cdot \frac{4}{3} \cdot \frac{4}{5} \cdot \frac{6}{5} \cdot \frac{6}{7} \cdots$$

Viète's formula has a nice geometric interpretation, and converges linearly. It gives about 2 bits (0.6 decimals) per term. Wallis's formula is more convenient, because of the lack of square roots, but converges more slowly (as you can see by taking logarithms of each side).

Continued fractions involving π

There are also *continued fractions* for π, e.g. Brouncker's

$$\frac{4}{\pi} = 1 + \cfrac{1^2}{2 + \cfrac{3^2}{2 + \cfrac{5^2}{2 + \cdots}}}$$

William Brouncker (1620–1684) was the first president of the Royal Society. He solved "Pell's equation" $x^2 - Dy^2 = 1$ before Pell. However, Bhaskara II (1114–1185) solved it much earlier, so it should be named after Bhaskara (or maybe Brahmagupta, who solved special cases even earlier), rather than Pell or Brouncker.

Equivalence of a sum and a continued fraction

Writing Brouncker's formula as a continued fraction for $\pi/4$, the convergents are given by partial sums of the Gregory/Leibniz formula for π, e.g.

$$\cfrac{1}{1+\cfrac{1^2}{2+\cfrac{3^2}{2}}} = 1 - \frac{1}{3} + \frac{1}{5}\,.$$

The general case follows by putting $a_n := (1-2n)/(1+2n)$ in Euler's identity

$$\begin{aligned} & a_0 + a_0 a_1 + \cdots + a_0 a_1 \cdots a_n \\ & \quad = a_0/(1 - a_1/(1 + a_1 - a_2/(1 + a_2 - \cdots a_n/(1 + a_n) \cdots))). \end{aligned}$$

Euler's identity can easily be proved by induction on n.

The BBP formula

In 1995, Simon Plouffe discovered the formula

$$\pi = \sum_{k=0}^{\infty} \left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6} \right) 2^{-4k}.$$

It is called the BBP formula since it was published in a paper by David Bailey, Peter Borwein and Simon Plouffe.

The BBP formula allows us to find the n-th digit (or a short block of digits near the n-th) in the binary representation of π faster (in practice, if not in theory), and using much less memory, than any known algorithm for computing (all of) the first n digits.

No such formula is known for base ten (i.e. decimal arithmetic).

Formulas involving π and the zeta function

The *Riemann zeta function* $\zeta(s)$ is defined by $\zeta(s) := \sum_{k=1}^{\infty} k^{-s}$ for $\Re(s) > 1$, and by analytic continuation for other $s \in \mathbb{C}\backslash\{0\}$. It satisfies the functional equation $\xi(s) = \xi(1-s)$, where

$$\xi(s) := \frac{1}{2}\pi^{-s/2} s(s-1)\Gamma(s/2)\zeta(s).$$

Euler found that

$$\zeta(2n) = (-1)^{n+1}\frac{B_{2n}(2\pi)^{2n}}{2(2n)!} \text{ for non-negative integers } n.$$

The *Bernoulli numbers* $B_{2n} \in Q$ ($B_0 = 1$, $B_2 = \frac{1}{6}$, $B_4 = -\frac{1}{30}, \cdots$) have a simple exponential generating function $x/(e^x - 1) - x/2$. Euler's formula shows that $\zeta(2n)/\pi^{2n}$ is a *rational* number. For example, $\zeta(2) = \pi^2/6$, $\zeta(4) = \pi^4/90$.

Generalisations

One reason why formulas involving π are interesting is that they can often be generalised. For example: $e^{i\pi} = -1$ is a special case of $e^{i\theta} = \cos\theta + i\sin\theta$.

$\sqrt{\pi} = \Gamma(\frac{1}{2})$ is a special case of $\sqrt{\pi} = 2^{2s-1}\frac{\Gamma(s)\Gamma(s+\frac{1}{2})}{\Gamma(2s)}$.

Euler's formula for $\zeta(2n)$ follows from the Hadamard product

$$\frac{\sin \pi z}{\pi z} = \prod_{n=1}^{\infty}\left(1 - \frac{z^2}{n^2}\right).$$

We'll later see examples involving elliptic integrals, theta functions, etc. Thus, a formula for π is often just the tip of a large iceberg!

Why do we need many digits of π?

To compute the circumference of the Earth to an accuracy of 1mm from the formula $2\pi r$, we only need π to 11 decimal digits. The circumference of the observable universe can be computed to within one Planck length (1.6×10^{-35} metres) if we know π to about 62 decimal digits, assuming that space-time is flat and we know the radius.

Hence, why would anyone ever be interested in computing π to more than 100 decimal digits?

One answer

One possible answer: because

$$e := \sum_{k=0}^{\infty} \frac{1}{k!}$$

is too easy, and Brun's constant

$$B := \sum_{p,\ p+2 \text{ prime}} \left(\frac{1}{p} + \frac{1}{p+2}\right)$$

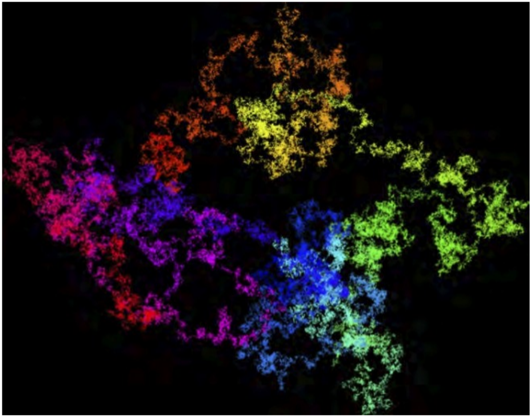
is too hard! We only know

$$1.84 < B < 2.29$$

(Platt and Trudgian, 2018).

Another answer

So we can draw pictures like this [Aragón, Bailey, Borwein et al]



This "walk" on the first 10^{11} base-4 digits of π suggests (but doesn't prove) that π is normal in base 4.

More answers

As we said already, π is the tip of an iceberg, and we want to see what is underwater.

To find identities using the PSLQ algorithm (Ferguson and Bailey) or to numerically verify conjectured identities, we need to be able to compute the relevant terms to high precision.

For example, the BBP algorithm was found in this way.

Thus, we want to be able to compute many constants to high precision, for example $\zeta(3)$, γ, $\Gamma(p/q)$ for rational p/q, $\exp(\pi\sqrt{163}) = 262537412640768743.99999999999992\cdots$, etc.

To implement arbitrary-precision software such as MPFR, we need algorithms for the computation of elementary and special functions to arbitrary precision.

Another answer

As in mountain-climbing, "because it is there!"

Of course, a mountain has a finite height, so in principle we can get to the top. $\pi = 3.14159265\cdots$ has a non-terminating (and non-periodic) decimal (or binary) expansion, so we can never compute all of it.

For this reason, it is more satisfying to work on algorithms for computing π than on programs that approximate it to a large (but finite) number of digits. I suspect that Jon Borwein had the same view, since he found some nice algorithms for π, but left it to collaborators to implement them.
In the rest of this talk we'll concentrate on algorithms for computing π. It would be more accurate to say "approximating" than "computing", since we can never compute the full (countably infinite) binary or decimal representation of π.

Some means

To refresh your memory, the *arithmetic mean* of $a, b \in \mathbb{R}$ is

$$\mathrm{AM}(a, b) := \frac{a+b}{2}\,.$$

The *geometric mean* is

$$\mathrm{GM}(a, b) := \sqrt{ab},$$

and the *harmonic mean* (for $ab \neq 0$) is

$$\mathrm{HM}(a, b) := \mathrm{AM}(a^{-1}, b^{-1})^{-1} = \frac{2ab}{a+b}\,.$$

Assuming that a and b are positive, we have the inequalities

$$\mathrm{HM}(a, b) \leq \mathrm{GM}(a, b) \leq \mathrm{AM}(a, b).$$

The arithmetic-geometric mean

Given two positive reals a_0, b_0, we can iterate the arithmetic and geometric means by defining, for $n \geq 0$,

$$\begin{aligned} a_{n+1} &= \mathrm{AM}(a_n, b_n) \\ b_{n+1} &= \mathrm{GM}(a_n, b_n). \end{aligned}$$

The sequences (a_n) and (b_n) converge to a common limit called the *arithmetic-geometric mean* (AGM) of a_0 and b_0. We denote it by $\mathrm{AGM}(a_0, b_0)$.

The harmonic-geometric mean

We could define an iteration

$$\begin{aligned} a_{n+1} &= \mathrm{HM}(a_n, b_n) \\ b_{n+1} &= \mathrm{GM}(a_n, b_n). \end{aligned}$$

However, we see that

$$\begin{aligned} a_{n+1}^{-1} &= \mathrm{AM}(a_n^{-1}, b_n^{-1}) \\ b_{n+1}^{-1} &= \mathrm{GM}(a_n^{-1}, b_n^{-1}). \end{aligned}$$

Thus, the common limit is just $\mathrm{AGM}(a_0^{-1}, b_0^{-1})^{-1}$.

Replacing the arithmetic mean by the harmonic mean in the definition of the AGM does not give anything essentially new.

Another mean

Note that $\mathrm{AGM}(a_0, b_0) = \mathrm{AGM}(b_0, a_0)$ is symmetric in a_0, b_0. This is not true if we use a slightly different iteration

$$\begin{aligned} a_{n+1} &= \mathrm{AM}(a_n, b_n) \\ b_{n+1} &= \mathrm{GM}(a_{n+1}, b_n) \end{aligned}$$

which converges to a limit which we denote by $\mathrm{ARM}(a_0, b_0)$ ("AR" for "Archimedes", as we'll explain shortly).

The ARM is slightly easier to implement in a program than the AGM, as we can just drop the subscripts and iterate $\{a := \mathrm{AM}(a, b);\ b := \mathrm{GM}(a, b)\}$, avoiding the use of a temporary variable.

Archimedes

Archimedes (c.287–c.212 BC) gave perhaps the first iterative algorithm for computing π to arbitrary precision, and used the first few iterations to show that

$$3.1408 \approx 3\tfrac{10}{71} < \pi < 3\tfrac{1}{7} \approx 3.1429\,.$$

Many people believe that $\pi = 3\frac{1}{7}$. Archimedes knew better.

Digression: a recent one-line proof that $\pi < 3\frac{1}{7}$ is

$$0 < \int_0^1 \frac{x^4(1-x)^4}{1+x^2}\,dx = \frac{22}{7} - \pi.$$

To evaluate the integral, write the integrand as

$$x^6 - 4x^5 + 5x^4 - 4x^2 + 4 - \frac{4}{1+x^2}$$

and integrate term by term, using

$$\int_0^1 \frac{dx}{1+x^2} = \arctan(1) = \frac{\pi}{4}.$$

Inscribed and circumscribed polygons

Archimedes' key idea is to use the perimeters of inscribed and circumscribed polygons in a circle of radius $1/2$ to give lower and upper bounds on π. We start with hexagons and keep bisecting angles to get polygons with $6 \cdot 2^n$ sides.

Let A_n denote the perimeter of a circumscribed regular $6 \cdot 2^n$-gon, and B_n ditto for the inscribed regular $6 \cdot 2^n$-gon. Writing $\ell_n := 6 \cdot 2^n$, $\theta_n := \frac{\pi}{\ell_n}$, we see that

$$B_n = \ell_n \sin \theta_n < \pi < A_n = \ell_n \tan \theta_n.$$

The initial values are $\ell_0 = 6, \theta_0 = \pi/6, A_0 = 2\sqrt{3}, B_0 = 3$. Using "half-angle" formulas we can verify that

$$\begin{aligned} A_{n+1} &= \mathrm{HM}(A_n, B_n), \\ B_{n+1} &= \mathrm{GM}(A_{n+1}, B_n). \end{aligned}$$

Archimedes continued

Recall that

$$\begin{aligned} A_{n+1} &= \mathrm{HM}(A_n, B_n), \\ B_{n+1} &= \mathrm{GM}(A_{n+1}, B_n). \end{aligned}$$

To avoid the harmonic mean, define $a_n := 1/A_n,\ b_n := 1/B_n$. Then

$$\begin{aligned} a_{n+1} &= \mathrm{AM}(a_n, b_n), \\ b_{n+1} &= \mathrm{GM}(a_{n+1}, b_n). \end{aligned}$$

This is just an instance of the "Archimedes mean" ARM defined previously, so we see that

$$\mathrm{ARM}\left(\frac{\sqrt{3}}{6}, \frac{1}{3}\right) = \frac{1}{\pi}\,.$$

Similar methods give

$$ARM(\cos\theta, 1) = \frac{\sin\theta}{\theta},\quad ARM(\cosh\theta, 1) = \frac{\sinh\theta}{\theta}\,.$$

Upper and lower bounds via Archimedes

Using Archimedes' method gives (correct digits in blue):

$$
\begin{aligned}
\text{iteration } 0: &\quad 3.0000000 < \pi < 3.4641017 \\
\text{iteration } 1: &\quad 3.1058285 < \pi < 3.2153904 \\
\text{iteration } 2: &\quad 3.1326286 < \pi < 3.1596600 \\
\text{iteration } 3: &\quad 3.1393502 < \pi < 3.1460863 \quad < 3.1464 \\
\text{iteration } 4: &\quad 3.1410319 < \pi < 3.1427146 \quad < 3.1435 \\
\text{iteration } 5: &\quad 3.1414524 < \pi < 3.1418731 \\
\text{iteration } 6: &\quad 3.1415576 < \pi < 3.1416628 \\
\text{iteration } 7: &\quad 3.1415838 < \pi < 3.1416102 \\
\text{iteration } 8: &\quad 3.1415904 < \pi < 3.1415971
\end{aligned}
$$

The bounds satisfy

$$A_n - B_n = \pi \left(\frac{\tan\theta_n - \sin\theta_n}{\theta_n} \right) < 2^{-2n-1}.$$

We get two bits of accuracy per iteration (linear convergence).

Implications of Archimedes' method

David Bailey has observed that there are at least *eight* recent papers in the "refereed" literature claiming that $\pi = (14 - \sqrt{2})/4 = 3.1464\cdots$, and another three claiming that $\pi = 17 - 8\sqrt{3} = 3.1435\cdots$.

These claims must be incorrect, due to Lindemann's 1882 theorem that π is transcendental, but we can give a more elementary disproof of the claims for anyone who does not understand Lindemann's proof.

Since $A_3 < 3.1464$ and $A_4 < 3.1435$, we see that four iterations of Archimedes' method suffice to disprove the claims.

Four iterations of Archimedes' method suffice to show that

$$3.1408 < 3\tfrac{10}{71} < \pi < 3\tfrac{1}{7} < 3.1429\,,$$

as (correctly) claimed by Archimedes.

What if Archimedes made a small change?

We've seen that the essential part of Archimedes' method is the iteration

$$\begin{aligned} a_{n+1} &= \mathrm{AM}(a_n, b_n), \\ b_{n+1} &= \mathrm{GM}(a_{n+1}, b_n). \end{aligned}$$

If Archimedes had written it this way, he might have considered making a small change and using the (more symmetric) iteration

$$\begin{aligned} a_{n+1} &= \mathrm{AM}(a_n, b_n), \\ b_{n+1} &= \mathrm{GM}(a_{n}, b_n). \end{aligned}$$

This is just the arithmetic-geometric mean!

What if $\cdots$ continued

Archimedes would have found that the new (AGM) iteration converges much faster than the old (ARM) iteration. To see this, suppose that $x_n := a_n/b_n = 1 + \varepsilon_n$. Then

$$x_{n+1} = \tfrac{1}{2}(a_n/b_n + 1)/\sqrt{a_n/b_n} = \tfrac{1}{2}(x_n^{1/2} + x_n^{-1/2}),$$

so

$$1 + \varepsilon_{n+1} = \tfrac{1}{2}((1+\varepsilon_n)^{1/2} + (1+\varepsilon_n)^{-1/2}) = 1 + \tfrac{1}{8}\varepsilon_n^2 + O(\varepsilon_n^3).$$

Thus $\varepsilon_{n+1} \approx \frac{1}{8}\varepsilon_n^2$ if $|\varepsilon_n|$ is small.

This is an example of *quadratic* convergence – the number of correct digits roughly doubles at each iteration. In contrast, the ARM has only *linear* convergence – the number of correct digits increases roughly linearly with each iteration.

The limit

Although the AGM iteration converges faster than the ARM iteration, it does not give the same limit. Thus, it's not immediately obvious that it is useful for computing π (or anything else of interest).

Gauss and Legendre solved the problem of expressing AGM(a, b) in terms of known functions. The answer may be written as

$$\frac{1}{\mathrm{AGM}(a,b)} = \frac{2}{\pi} \int_0^{\pi/2} \frac{d\theta}{\sqrt{a^2 \cos^2\theta + b^2 \sin^2\theta}} .$$

The right-hand-side is the product of a constant (whose precise value will be significant later) and a *complete elliptic integral*.

Elliptic integrals

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

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

and the *complete elliptic integral of the second kind* by

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

The variable k is called the *modulus*, and $k' := \sqrt{1-k^2}$ is called the *complementary modulus*.

Some (confusing) notation

It is customary to define

$$K'(k) := K(\sqrt{1-k^2}) = K(k')$$

and

$$E'(k) := E(\sqrt{1-k^2}) = E(k'),$$

so in the context of elliptic integrals a prime (′) does *not* denote differentiation. Apologies for any confusion, but this is the convention that is used in the literature, including *Pi and the AGM*.

On the rare occasions when we need a derivative, we use operator notation $\mathrm{D}_k K(k) := dK(k)/dk$.

Pi and the AGM uses the "dot" notation $\dot{K}(k) := dK(k)/dk$, but this is confusing and hard to see, so we'll avoid it.

k and k' can in general be complex, but in this talk we'll assume that they are real and in the interval $(0, 1)$.

What's in a name?

The arc-length L of an ellipse with semi-major axis a and semi-minor axis b is given by

$$L = 4\int_0^{\pi/2} \sqrt{a^2\cos^2\theta + b^2\sin^2\theta}\, d\theta = 4aE'(b/a).$$

elliptic functions arise by inverting (incomplete) elliptic integrals.

elliptic curves are named because of their connection with elliptic functions.

...

ellipsis comes from the same Greek word, meaning “leave out” or “defective” (ellipses are defective circles).

Connection with hypergeometric functions

In terms of the Gaussian hypergeometric function

$$F(a,b;c;z) := 1 + \frac{a \cdot b}{1! \cdot c}\, z + \frac{a(a+1)\cdot b(b+1)}{2! \cdot c(c+1)}\, z^2 + \cdots$$

we have

$$K(k) = \frac{\pi}{2}\, F\left(\tfrac{1}{2}, \tfrac{1}{2}; 1; k^2\right)$$

and

$$E(k) = \frac{\pi}{2}\, F\left(-\tfrac{1}{2}, \tfrac{1}{2}; 1; k^2\right).$$

We also have

$$K'(k) = \frac{2}{\pi} \log\left(\frac{4}{k}\right) K(k) - f(k),$$

where $f(k) = k^2/4 + O(k^4)$ is analytic in the disk $|k| < 1$.
Note: in this talk, $\log$ always denotes the natural logarithm.

The AGM and elliptic integrals

Substituting $(a, b) \mapsto (1, k)$ above, and recalling that $k^2 + (k')^2 = 1$, we have

$$\begin{aligned}\frac{1}{\mathrm{AGM}(1,k)} &= \frac{2}{\pi}\int_0^{\pi/2} \frac{d\theta}{\sqrt{\cos^2\theta + k^2\sin^2\theta}} \\ &= \frac{2}{\pi}\int_0^{\pi/2} \frac{d\theta}{\sqrt{1-(1-k^2)\sin^2\theta}} \\ &= \frac{2}{\pi}\int_0^{\pi/2} \frac{d\theta}{\sqrt{1-(k')^2\sin^2\theta}} \\ &= \frac{2}{\pi}K'(k),\end{aligned}$$

so

$$\mathrm{AGM}(1,k) = \frac{\pi}{2K'(k)}\,.$$

Computing both E' and K' via the AGM

We have seen that, if we start from $a_0 = 1$, $b_0 = k \in (0,1)$ and apply the AGM iteration, then $K'(k)$ can be computed from

$$\lim_{n\to\infty} a_n = \frac{\pi}{2K'(k)} \cdot$$

We also have

$$\frac{E'(k)}{K'(k)} = \frac{1+k^2}{2} - \sum_{n=0}^{\infty} 2^n \left(a_n - a_{n+1}\right)^2,$$

so $E'(k)$ can be computed at the same time as $K'(k)$.

Logarithms and the AGM

Recall that, for small k, we have

$$K'(k) = \frac{2}{\pi} \log\left(\frac{4}{k}\right) K(k) + O(k^2),$$

but

$$\frac{2}{\pi} K(k) = F\left(\tfrac{1}{2}, \tfrac{1}{2}; 1; k^2\right) = 1 + O(k^2).$$

Thus, assuming that $k \in (0, 1)$, we have

$$K'(k) = \left(1 + O(k^2)\right) \log\left(\frac{4}{k}\right).$$

An explicit bound on the $O(k^2)$ term is given in Thm. 7.2 of *Pi and the AGM*.

First attempt to compute π via the AGM

Choose $k := 2^{2-n}$ for some sufficiently large positive integer n. Then

$$\log\left(\frac{4}{k}\right) = n\log 2,$$

but

$$\frac{\pi}{2\,\mathrm{AGM}(1,k)} = K'(k) = \left(1 + O(k^2)\right)\log\left(\frac{4}{k}\right),$$

which gives

$$\frac{\pi}{\log 2} = 2n\,\mathrm{AGM}(1,k)\ \left(1 + O(4^{-n})\right).$$

Thus, we can compute $\pi/\log 2$ to $(2n + O(1))$-bit accuracy using an AGM computation. Similarly for $\pi/\log 3$, etc.

Historical notes

The algorithm for $\pi/\log 2$ was essentially given by Salamin in HAKMEM (1972), pg. 71, although presented as an algorithm for computing $\log(4/k)$, assuming that we know π.

On the same page Salamin gives an algorithm for computing π, taking $k = 4/e^n$ instead of our $k = 4/2^n$. With his choice $\pi \approx 2n\,\mathrm{AGM}(1, k)$. However, this assumes that we know e, so it is not a "standalone" algorithm for π via the AGM.

In 1975, Salamin (and independently the speaker) discovered an algorithm for computing π via the AGM *without* needing to know e or $\log 2$ to high precision. It is called the "Gauss-Legendre" or "Brent-Salamin" algorithm, and is about twice as fast as the algorithm given in HAKMEM (1972).

In 1984, Jon and Peter Borwein discovered another quadratically convergent algorithm for computing π, with about the same speed as the Gauss-Legendre algorithm. We'll describe the Gauss-Legendre and Borwein-Borwein algorithms shortly.

Legendre's relation

The Gauss-Legendre algorithm takes advantage of a nice identity known as *Legendre's relation*: for $0 < k < 1$,

$$E(k)K'(k) + E'(k)K(k) - K(k)K'(k) = \frac{\pi}{2} \cdot$$

For a proof, see *Pi and the AGM*, Sec. 1.6.

A quadratically convergent algorithm for π

Using Legendre's relation and the formulas that we've given for E and K in terms of the AGM iteration, it is not difficult to derive the **Gauss-Legendre** algorithm.

Set $a_0 = 1$, $b_0 = 1/\sqrt{2}$, $s_0 = \frac{1}{4}$ and iterate (for $n = 0, 1, \ldots$)

$$a_{n+1} = \frac{a_n + b_n}{2}, \;\; b_{n+1} = \sqrt{a_n b_n}, \;\; s_{n+1} = s_n - 2^n (a_n - a_{n+1})^2.$$

Then we get upper and lower bounds on π:

$$\frac{a_n^2}{s_n} > \pi > \frac{a_{n+1}^2}{s_n},$$

and both bounds converge quadratically to π. The lower bound is more accurate, so the algorithm is often stated with just the lower bound a_{n+1}^2/s_n.

Gauss and Legendre

Louis Legendre (1752-1797) politician
unrelated to the mathematician

How fast does it converge?

n	a_{n+1}^2/s_n				a_n^2/s_n
0 :	2.914213562373095048801689	$<$	π	$<$	4.000000000000000000000000
1 :	3.140579250522168248311331	$<$	π	$<$	3.187672642712108627201930
2 :	3.141592646213542282149344	$<$	π	$<$	3.141680293297653293918070
3 :	3.141592653589793238279513	$<$	π	$<$	3.141592653895446496002915
4 :	3.141592653589793238462643	$<$	π	$<$	3.141592653589793238466361

Compare Archimedes:

$$0: \; 3.0000000 < \pi < 3.4641017$$
$$1: \; 3.1058285 < \pi < 3.2153904$$
$$2: \; 3.1326286 < \pi < 3.1596600$$
$$3: \; 3.1393502 < \pi < 3.1460863$$
$$4: \; 3.1410319 < \pi < 3.1427146$$
$$\cdots$$
$$37: \; 3.141592653589793238462636 < \pi < 3.141592653589793238462659$$

Jacobi theta functions

To estimate the speed of convergence and, more precisely, to obtain upper and lower bounds on the error after n iterations, we consider the parameterisation of the AGM in terms of *Jacobi theta functions*.

Theta functions and the AGM

We need the basic theta functions of one variable defined by

$$\theta_3(q) := \sum_{n\in\mathbb{Z}} q^{n^2}, \;\; \theta_4(q) := \sum_{n\in\mathbb{Z}} (-1)^n q^{n^2}, \;\; |q| < 1.$$

It is not difficult to show that

$$\frac{\theta_3^2(q) + \theta_4^2(q)}{2} = \theta_3^2(q^2) \;\text{ and }\; \sqrt{\theta_3^2(q)\theta_4^2(q)} = \theta_4^2(q^2).$$

This shows that the AGM variables (a_n, b_n) can, if scaled suitably, be parameterised by $(\theta_3^2(q^{2^n}), \theta_4^2(q^{2^n}))$.

Theta functions and the AGM

If $1 = a_0 > b_0 = \theta_4^2(q)/\theta_3^2(q) > 0$, where $q \in (0, 1)$, then the variables a_n, b_n appearing in the AGM iteration satisfy

$$a_n = \frac{\theta_3^2(q^{2^n})}{\theta_3^2(q)}\,, \;\; b_n = \frac{\theta_4^2(q^{2^n})}{\theta_3^2(q)}\,.$$

We can write q (which is called the *nome*) explicitly in terms of the elliptic integral K with $k' = b_0/a_0$, in fact

$$q = \exp(-\pi K'(k)/K(k)).$$

This is due to Gauss/Jacobi.

An efficient special case is $k = k` = 1/\sqrt{2}$. Then $K' = K$ and

$$q = e^{-\pi} = 0.0432139\ldots$$

Theta functions and the AGM

Recall that in the Gauss-Legendre algorithm we have $a_0 = 1$, $b_0 = 1/\sqrt{2}$, $s_0 = \frac{1}{4}$ and, for $n \ge 0$,

$$a_{n+1} = \frac{a_n + b_n}{2}, \;\; b_{n+1} = \sqrt{a_n b_n}, \;\; s_{n+1} = s_n - 2^n (a_n - a_{n+1})^2.$$

Take $q = e^{-\pi}$, and write

$$a_\infty := \lim_{n\to\infty} a_n = \theta_3^{-2}(q) = 2\pi^{3/2}/\Gamma^2(\tfrac{1}{4}) \approx 0.8472,$$
$$s_\infty := \lim_{n\to\infty} s_n = \theta_3^{-4}(q)/\pi = 4\pi^2/\Gamma^4(\tfrac{1}{4}) \approx 0.2285\,.$$

It is curious that the algorithm computes π as the ratio of a_∞^2 and s_∞, both of which appear more "complicated" than π.

As on the previous slide, $a_n = \theta_3^2(q^{2^n})/\theta_3^2(q)$, and thus

$$s_n - s_\infty = \theta_3^{-4}(q) \sum_{m=n}^{\infty} 2^m \left(\theta_3^2(q^{2^m}) - \theta_3^2(q^{2^{m+1}})\right)^2.$$

Simplification

The expression for $s_n - s_\infty$ can be simplified if we use the theta function

$$\theta_2(q) := \sum_{n\in\mathbb{Z}} q^{(n+1/2)^2}.$$

Jacobi's identity

$$\theta_3^4(q) = \theta_2^4(q) + \theta_4^4(q)$$

connects θ_2, θ_3 and θ_4. Using it, we see that

$$s_n - s_\infty = \theta_3^{-4}(q) \sum_{m=n}^{\infty} 2^m \theta_2^4(q^{2^{m+1}}).$$

Theta functions and the AGM

Write $a_n/a_\infty = 1 + \delta_n$ and $s_n/s_\infty = 1 + \varepsilon_n$. Then

$$\delta_n = \theta_3^2(q^{2^n}) - 1 \sim 4q^{2^n} \;\text{ as }\; n \to \infty,$$

and

$$\varepsilon_n \sim \pi\, 2^n\, \theta_2^4(q^{2^{n+1}}) \sim 2^{n+4}\pi q^{2^{n+1}}.$$

Upper and lower bounds

Writing

$$\frac{a_n^2/a_\infty^2}{s_n/s_\infty} = \frac{a_n^2}{\pi s_n} = \frac{(1+\delta_n)^2}{1+\varepsilon_n}\,,$$

it is straightforward to obtain an upper bound on π:

$$0 < a_n^2/s_n - \pi < U(n) := 8\pi q^{2^n}.$$

Convergence is quadratic: if $e_n := a_n^2/s_n - \pi$, then

$$\lim_{n\to\infty} e_{n+1}/e_n^2 = \tfrac{1}{8\pi}\,\cdot$$

Replacing a_n by a_{n+1} and δ_n by δ_{n+1}, we obtain a lower bound (after $n+1$ square roots)

$$0 < \pi - \frac{a_{n+1}^2}{s_n} < L(n) := (2^{n+4}\pi^2 - 8\pi)q^{2^{n+1}}.$$

Numerical values of upper and lower bounds

n	$a_n^2/s_n - \pi$	$\pi - a_{n+1}^2/s_n$	$\frac{a_n^2/s_n-\pi}{U(n)}$	$\frac{\pi-a_{n+1}^2/s_n}{L(n)}$
0	8.58e-1	2.27e-1	0.790369040	0.916996189
1	4.61e-2	1.01e-3	0.981804947	0.999656206
2	8.76e-5	7.38e-9	0.999922813	0.999999998
3	3.06e-10	1.83e-19	0.999999999	1.000000000
4	3.72e-21	5.47e-41	1.000000000	1.000000000
5	5.50e-43	2.41e-84	1.000000000	1.000000000
6	1.20e-86	2.31e-171	1.000000000	1.000000000
7	5.76e-174	1.06e-345	1.000000000	1.000000000
8	1.32e-348	1.11e-694	1.000000000	1.000000000

$U(n) := 8\pi\exp(-2^n\pi)$ and $L(n) := (2^{n+4}\pi^2 - 8\pi)\exp(-2^{n+1}\pi)$ are the bounds given above. It can be seen that they are very accurate, as expected from our analysis.

The Borwein^2 quadratic AGM algorithm for π

In *Pi and the AGM*, Jon and Peter Borwein present a *different* quadratically convergent algorithm for π based on the AGM. (It is Algorithm 2.1 in Chapter 2, and was first published in 1984.)

Instead of using Legendre's relation, the Borwein-Borwein algorithm uses the identity

$$K(k)\,\mathrm{D}_k K(k)\big|_{k=1/\sqrt{2}} = \frac{\pi}{\sqrt{2}}\,,$$

where D_k denotes differentiation with respect to k.

Using the connection between $K(k')$ and the AGM, we obtain

$$\pi = 2^{3/2}\,\frac{(\mathrm{AGM}(1,k'))^3}{\mathrm{D}_k\,\mathrm{AGM}(1,k')}\bigg|_{k=1/\sqrt{2}}\,.$$

An algorithm for approximating the derivative in this formula can be obtained by differentiating the AGM iteration symbolically. Details are given in *Pi and the AGM*.

The Borwein^2 quadratic AGM algorithm for π

The Borwein-Borwein algorithm (Alg. 2.1 of *Pi and the AGM*):

$$x_0 := \sqrt{2};\;\; y_1 := 2^{1/4};\;\; \underline{\pi}_0 := \sqrt{2};\;\; \overline{\pi}_0 := 2 + \sqrt{2};$$

$$\text{for } n \ge 0,\ x_{n+1} := \tfrac{1}{2}(x_n^{1/2} + x_n^{-1/2});$$

$$\text{for } n \ge 1,\ y_{n+1} := \frac{y_n x_n^{1/2} + x_n^{-1/2}}{y_n + 1};$$

$$\text{for } n \ge 1,\ \underline{\pi}_n := \frac{2\,\overline{\pi}_{n-1}}{y_n + 1},\ \ \overline{\pi}_n := \underline{\pi}_n \left(\frac{x_n + 1}{2} \right).$$

Then $\overline{\pi}_n$ decreases monotonically to π, and $\underline{\pi}_n$ increases monotonically to π. (The algorithm given in *Pi and the AGM* defines $\overline{\pi}_n := \overline{\pi}_{n-1}(x_n + 1)/(y_n + 1)$ and omits $\underline{\pi}_n$.)

The AGM iteration is present in *Legendre form*: if $a_0 := 1$, $b_0 := k' = 1/\sqrt{2}$, and we perform the AGM iteration, then $x_n = a_n/b_n$ and, for $n \ge 1$, $y_n = \mathrm{D}_k b_n/\mathrm{D}_k a_n$.

How fast does Borwein-Borwein converge?

n	$\underline{\pi}_n$		$\overline{\pi}_n$
0 :	1.414213562373095048801689	$< \pi <$	3.414213562373095048801689
1 :	3.11913252882772757303373	$< \pi <$	3.142606753941622600790720
2 :	3.141548837729436193482357	$< \pi <$	3.141592660966044230497752
3 :	3.141592653436966609787790	$< \pi <$	3.141592653589793238645774
4 :	3.141592653589793238460785	$< \pi <$	3.141592653589793238462643

Compare **Gauss-Legendre:**

n	a_{n+1}^2/s_n		a_n^2/s_n
0 :	2.914213562373095048801689	$< \pi <$	4.00000000000000000000000
1 :	3.140579250522168248311331	$< \pi <$	3.187672642712108627201930
2 :	3.141592646213542282149344	$< \pi <$	3.141680293297653293918070
3 :	3.141592653589793238279513	$< \pi <$	3.141592653895446496002915
4 :	3.141592653589793238462643	$< \pi <$	3.141592653589793238466361

Borwein-Borwein gives better upper bounds, but worse lower bounds, for the same value of n (i.e. same number of sqrts).

Bounding the error using theta functions

As for the Gauss-Legendre algorithm, we can express the error after n iterations of the Borwein-Borwein algorithm using theta functions, and deduce the asymptotic behaviour of the error.

The result is an upper bound (for $n \geq 1$)

$$0 < \overline{\pi}_n - \pi < 2^{n+4}\pi^2 q^{2^{n+1}},$$

and a lower bound

$$0 < \pi - \underline{\pi}_n < 4\pi q^{2^n},$$

where $q = e^{-\pi}$.

These can be compared with the *lower bound* $2^{n+4}\pi^2 q^{2^{n+1}}$ and *upper bound* $8\pi q^{2^n}$ for the Gauss-Legendre algorithm.

Numerical values of upper and lower bounds

n	$\overline{\pi} - \pi$	ratio to bound	$\pi - \underline{\pi}$	ratio to bound
1	1.01e-3	0.9896487063	2.25e-2	0.9570949132
2	7.38e-9	0.9948470082	4.38e-5	0.9998316841
3	1.83e-19	0.9974691480	1.53e-10	0.9999999988
4	5.47e-41	0.9987456847	1.86e-21	1.0000000000
5	2.41e-84	0.9993755837	2.75e-43	1.0000000000
6	2.31e-171	0.9996884727	6.01e-87	1.0000000000
7	1.06e-345	0.9998444059	2.88e-174	1.0000000000
8	1.11e-694	0.9999222453	6.59e-349	1.0000000000

It can be seen that the bounds are very accurate (as expected from the exact expressions for the errors in terms of theta functions). The upper bound overestimates the error by a factor of $1 + O(2^{-n})$.

A fourth-order algorithm for π

The Borwein brothers did not stop at quadratic (second-order) algorithms for π. In Chapter 5 of *Pi and the AGM* they gave algorithms of orders 3, 4, 5 and 7. Here is a nice iteration of order 4. It can be derived using a modular identity of order 4.

$$
\begin{aligned}
y_0 &:= \sqrt{2} - 1; \quad a_0 := 2y_0^2; \\
y_{n+1} &:= \frac{1 - (1 - y_n^4)^{1/4}}{1 + (1 - y_n^4)^{1/4}}; \\
a_{n+1} &:= a_n(1 + y_{n+1})^4 - 2^{2n+3} y_{n+1}(1 + y_{n+1} + y_{n+1}^2).
\end{aligned}
$$

Then $\pi_n := 1/a_n$ converges quartically to π, i.e. the number of correct digits is multiplied by (approximately) 4 each iteration!

An error bound is

$$0 < \pi - \pi_n < 4\pi^2\, 4^{n+1} \exp(-2\pi\, 4^n).$$

Convergence of the quartic algorithm

The table shows the error $\pi - \pi_n$ after n iterations of the Borwein quartic algorithm, and the ratio

$$\frac{\pi - \pi_n}{4\pi^2\, 4^{n+1} \exp(-2\pi\, 4^n)}$$

of the error to the upper bound given on the previous slide.

n	$\pi - \pi_n$	$(\pi - \pi_n)/\text{bound}$
0	2.273790912e-1	0.7710517124
1	7.376250956e-9	0.9602112619
2	5.472109145e-41	0.9900528160
3	2.308580715e-171	0.9975132040
4	1.110954934e-694	0.9993783010
5	9.244416653e-2790	0.9998445753
6	6.913088685e-11172	0.9999611438
7	3.376546688e-44702	0.9999902860
8	3.002256862e-178825	0.9999975715

Remark on efficiency

A higher-order algorithm is not necessarily more efficient than a quadratically convergent algorithm. We have to take the work per iteration into account. For a fair comparison, we can use Ostrowski's *efficiency index*, defined as

$$E := \frac{\log p}{W},$$

where $p > 1$ is the order of convergence and W is the work per iteration.

For example, three iterations of a quadratic algorithm can be combined to give an order 8 algorithm with three times the work per iteration. The efficiency index is the same in both cases, as it should be.

An observation

After $2n$ iterations of the Gauss-Legendre algorithm we have an (accurate) error bound

$$0 < \pi - a_{2n+1}^2/s_{2n} < 4\pi^2\, 4^{n+1} \exp(-2\pi\, 4^n).$$

This is the same as the (accurate) error bound

$$0 < \pi - \pi_n < 4\pi^2\, 4^{n+1} \exp(-2\pi\, 4^n);$$

for the Borwein quartic algorithm!

On closer inspection we find that the two algorithms (Gauss-Legendre “doubled” and Borwein quartic) are *equivalent*, in the sense that they give *exactly* the same sequence of approximations to π. This observation seems to be new – it is not stated in *Pi and the AGM* or in any of the relevant references that I have looked at.

Numerical verification

Here k is the number of square roots, and "$\pi -$ approximation" is the error in the approximation given by the Gauss-Legendre algorithm after $k - 1$ iterations, or by the Borweins' quartic algorithm after $(k - 1)/2$ iterations. The error is the same for both algorithms (computed to 1000 decimal digits).

k	$\pi -$ approximation
1	2.2737909121669818966095465906980480562749752399816e-1
3	7.3762509563132989512968071098827321760295030264154e-9
5	5.4721091456899418327485331789641785565936917028248e-41
7	2.3085807149343902668213207343869568303303472423996e-171
9	1.1109549335576998257002904117322306941479378545140e-694

Verification continued

For example, the first line of the table follows from

$$a_1^2/s_0 = \pi_0 = \frac{3}{2} + \sqrt{2}$$
$$\approx \pi - 0.227$$

and the second line follows from

$$a_3^2/s_2 = \pi_1 = \frac{(2^{-2} + 2^{-5/2} + 2^{-5/4} + \sqrt{2^{-5/4} + 2^{-7/4}})^2}{2^{3/4} + 2^{1/4} - 2^{-1/2} - \frac{5}{4}}$$
$$\approx \pi - 7.376... \times 10^{-9}.$$

Clearly this method of proof does not generalise. An inductive proof is given in my arXiv paper (arXiv:1802.07558).

Some amazing series (and fast algorithms) for π

Let $(x)_n := x(x+1)\cdots(x+n-1)$ denote the *ascending factorial*. In Chapter 5 of *Pi and the AGM*, Jon and Peter Borwein discuss *Ramanujan-Sato* series such as

$$\frac{1}{\pi} = 2^{3/2}\sum_{n=0}^{\infty}\frac{(\frac{1}{4})_n(\frac{1}{2})_n(\frac{3}{4})_n}{(n!)^3}\,\frac{(1103+26390n)}{99^{4n+2}}\,.$$

This series is linearly convergent, but adds nearly eight decimal digits per term, since $99^4 \approx 10^8$.

A more extreme example is the Chudnovsky series

$$\frac{1}{\pi} = 12\sum_{n=0}^{\infty}(-1)^n\,\frac{(6n)!\,(13591409+545140134n)}{(3n)!\,(n!)^3\,640320^{3n+3/2}}\,,$$

which adds about 14 decimal digits per term.

Complexity of computing elementary functions

It turns out that all the elementary functions can be computed to n-bit accuracy in the same time as π, up to a moderate constant factor. In other words, they all have bit-complexity $O(M(n)\log n)$, where $M(n) = O(n \log n \log\log n)$ is the bit-complexity of n-bit multiplication. (The $\log\log n$ here can be improved.)

A key idea is to use the AGM (with complex arguments) to compute the (principal value of) the complex log function, and Newton's method to compute inverse functions. We can compute all the usual "elementary" functions using

$$\exp(ix) = \cos x + i \sin x \ \text{ or } \ \Im \log(1 + ix) = \arctan(x)$$

combined with Newton's method and elementary identities. There is no time to talk about this in detail today. See my arXiv paper and Chapter 6 of *Pi and the AGM* for further details.

Conclusion

I hope that I have given you some idea of the mathematics contained in the book *Pi and the AGM*. In the time available I have only been able to cover a small fraction of the gems that can be discovered there.

It is not an "easy read", but it is a book that you can put under your pillow, like Dirichlet is said to have done with his copy of Gauss's *Disquisitiones Arithmeticae*.

Although the research covered in *Pi and the AGM* is only a small fraction of Jon's legacy, it is the part that overlaps most closely with my own research, which is why I decided to talk about it today, on "π day".

Jon and Peter Borwein, 2008

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