Computing $\pi$: A Light Lunchtime Entertainment

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$\pi$ day this year: 03/14/15 9:26:53

https://www.flickr.com/photos/ludiecochrane/3353934854/
Modern machines: $10^9$ approximate computations per second.

Make sure this isn’t $10^9$ mistakes per second!
Floating point is mostly *binary scientific notation*. Example:

\[
\frac{1}{5} = 0.2_{10} = (0.00110)_2 \\
= (1.1001100)_2 \times 2^{-3}
\]

- IEEE double rounds after 53 binary digits (≈ 16 decimal digits).
- Rule: *exact result, correctly rounded* for basic ops
- What happens when I do a sequence of steps?
Suppose bold digits are correct:

\[
\begin{align*}
1.093752543 & - 1.093741233 = 0.000011310
\end{align*}
\]

Inputs have six correct digits. Output has only one!
Example: Quadratic equations

How would you compute the smaller root of

\[ z^2 - z + \frac{\epsilon}{4} = 0? \]
Example: Quadratic equations

How would you compute the smaller root of

$$z^2 - z + \epsilon/4 = 0?$$

Quadratic formula:

$$z_{\pm} = \frac{1}{2} \left( 1 \pm \sqrt{1 - \epsilon} \right)$$

When $\epsilon$ is small, smaller root loses many digits to cancellation!
Example: Quadratic equation

How would you compute the smaller root of

\[ z^2 - z + \epsilon/4 = 0? \]

Quadratic formula:

\[ z = \frac{1}{2} \left( 1 \pm \sqrt{1 - \epsilon} \right) \]

Product of roots is \( \epsilon/4 \), so

\[ z_- = \frac{\epsilon/4}{z_+} = \frac{\epsilon}{2 \left( 1 + \sqrt{1 - \epsilon} \right)} \]

Accurate even for small \( \epsilon \)! But if \( z_- \approx 0 \), why care about correct digits?
What’s $\pi$ to ten digits?

If you couldn’t look it up, how would you figure it out?
Archimedes method
Archimedes method
Archimedes method

Move from a $2^k$ to a $2^{k+1}$-gon:

For a $2^k$-gon, define

- $\theta_k = \pi / 2^k$
- Half side length $h_k = \sin(\theta_k)$
- Semi-perimeter $s_k = 2^k h_k = 2^k \sin(\pi / 2^k) \to \pi$
Trig ensues

Recall:

\[ \sin(2\alpha) = 2 \sin(\alpha) \cos(\alpha) \]

Hence

\[
\sin^2(\theta_k) = 4 \sin^2(\theta_{k+1}) \cos^2(\theta_{k+1}) \\
= 4 \left( \sin^2(\theta_{k+1}) - \sin^4(\theta_{k+1}) \right)
\]

Get that \( h_{k+1}^2 = \sin^2(\theta_{k+1}) \) is the smaller root of

\[
z^2 - z + \frac{h_k^2}{4} = 0.
\]

We know the quadratic formula, right?

\[
h_{k+1}^2 = \frac{1}{2} \left( 1 - \sqrt{1 - h_k^2} \right)
\]
Computing \( \pi \), take 1

Compute half-side-lengths by recurrence:

\[
\begin{align*}
    h_2^2 &= 1/2 \\
    h_{k+1}^2 &= \frac{1}{2} \left( 1 - \sqrt{1 - h_k^2} \right)
\end{align*}
\]

Then use

\[
\pi \approx 2^k h_k
\]
Uh-oh

At $k = 30$, computer claim $s_k = 0$!
Computing $\pi$, take 2

Problematic formula:

$$h_{k+1}^2 = \frac{1}{2} \left( 1 - \sqrt{1 - h_k^2} \right)$$

We know how to fix this!

$$h_{k+1}^2 = \frac{h_k^2}{2 \left( 1 + \sqrt{1 - h_k^2} \right)}$$
A Turn of the Screw

Better

\[ |\hat{s}_k - \pi| \]

- \( \hat{s}_k \)
- \( \pi \)

- Bad
- Good

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Outline

1. Innocuous Errors?
2. A Turn of the Screw
3. Awesome Acceleration
4. Beyond Pi
Model Madness
Convergence looks very systematic. In fact

\[ 2^k h_k = 2^k \left( 2^{-k} \pi - \frac{1}{6} (2^{-k} \pi)^3 + \ldots \right) \]

\[ = \pi - \frac{\pi^3}{6} 2^{-2k} + O(2^{-4k}) \]

The error at step \( k \) is about four times the error at step \( k + 1 \).
If $e_k$ is the error at step $k$, then

$$s_k = \pi + e_k$$

$$s_{k+1} = \pi + e_k/4 + \epsilon$$

Combine:

$$s'_{k+1} = \frac{4s_{k+1} - s_k}{3} = \pi + \epsilon$$

Rinse, wash, repeat!
Accelerated Convergence

![Graph showing error convergence over iterations](image)

- $s$
- $s'$
- $s''$
- $s'''$

Error vs. $k$
Another formula for $\pi$:

$$\pi = 4 \arctan(1) = 4 \left( 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \ldots \right)$$

Converges very slowly – $\approx 5 \times 10^5$ terms for six-digit accuracy.

I want to accelerate... but don’t have an error expansion!
Shanks Transformation

Suppose partial sum $s_k$ has error $e_k \approx \alpha q^k$.

\[
s_{k-1} \approx A + \alpha q^{k-1}
\]
\[
s_k \approx A + \alpha q^k
\]
\[
s_{k+1} \approx A + \alpha q^{k+1}
\]

Have

\[
q \approx \frac{s_{k+1} - s_k}{s_k - s_{k-1}}, \quad A \approx \frac{q^{-1}s_{k+1} - s_k}{q^{-1} - 1}
\]

Combine and do some algebra:

\[
s'_{k+1} = \frac{s_{k+1}s_{k-1} - s_k^2}{s_{k+1} - 2s_k + s_{k-1}}.
\]
Shanks again
A couple iterations of Shanks helps a lot

Things start disintegrating with a couple more steps

Why? Transformation formula is prone to cancellation!

Problems can be mitigated (not removed) with some cleverness
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Accelerating Past Pi

Same acceleration techniques are used...

- To solve linear systems (Krylov subspace methods)
  - Formally equivalent to Shanks and related transforms
  - We usually don’t think of it that way
  - Different perspective helps with stability!
  - Some of my research involves these ideas

- To solve nonlinear systems (Anderson acceleration)
  - Used for many years in computational quantum mech (DFT)
  - Recently back in vogue for more general nonlinear systems

Many opportunities for new twists on old ideas.
I have no idea what you're talking about...

...so here's a bunny with a pancake on its head.