Computing π: A Light Lunchtime Entertainment

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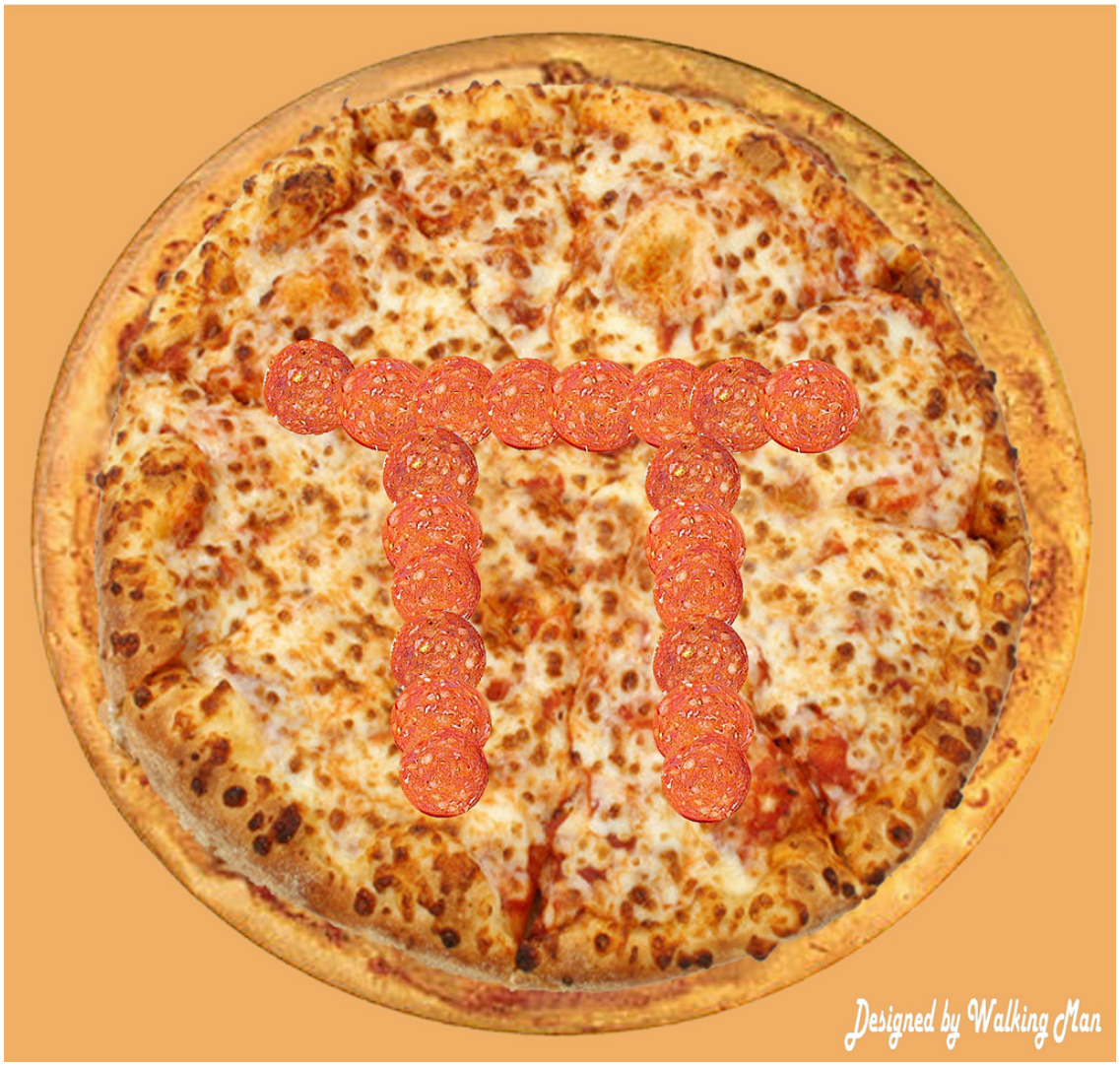
π day this year: 03/14/15 9:26:53



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Outline

1. Innocuous Errors?
2. A Turn of the Screw
3. Awesome Acceleration
4. Beyond Pi

Lies My Calculator Told Me

Modern machines: 10^9 approximate computations per second.

Make sure this isn't 10^9 *mistakes* per second!

Binary floating point

Floating point is mostly *binary scientific notation*. Example:

$$\frac{1}{5} = 0.2_{10} = (0.0\overline{0110})_2$$
$$= (1.100\overline{1100})_2 \times 2^{-3}$$

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

Cancellation

Suppose bold digits are correct:

$$
\begin{array}{rl}
 & \mathbf{1.09375}2543 \\
- & \mathbf{1.09374}1233 \\
\hline
= & \mathbf{0.00001}1310
\end{array}
$$

Inputs have six correct digits. Output has only one!

Example: Quadratic equations

How would you compute the smaller root of

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

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Quadratic formula:

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

When ϵ 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 ϵ! But if $z_- \approx 0$, why care about correct digits?

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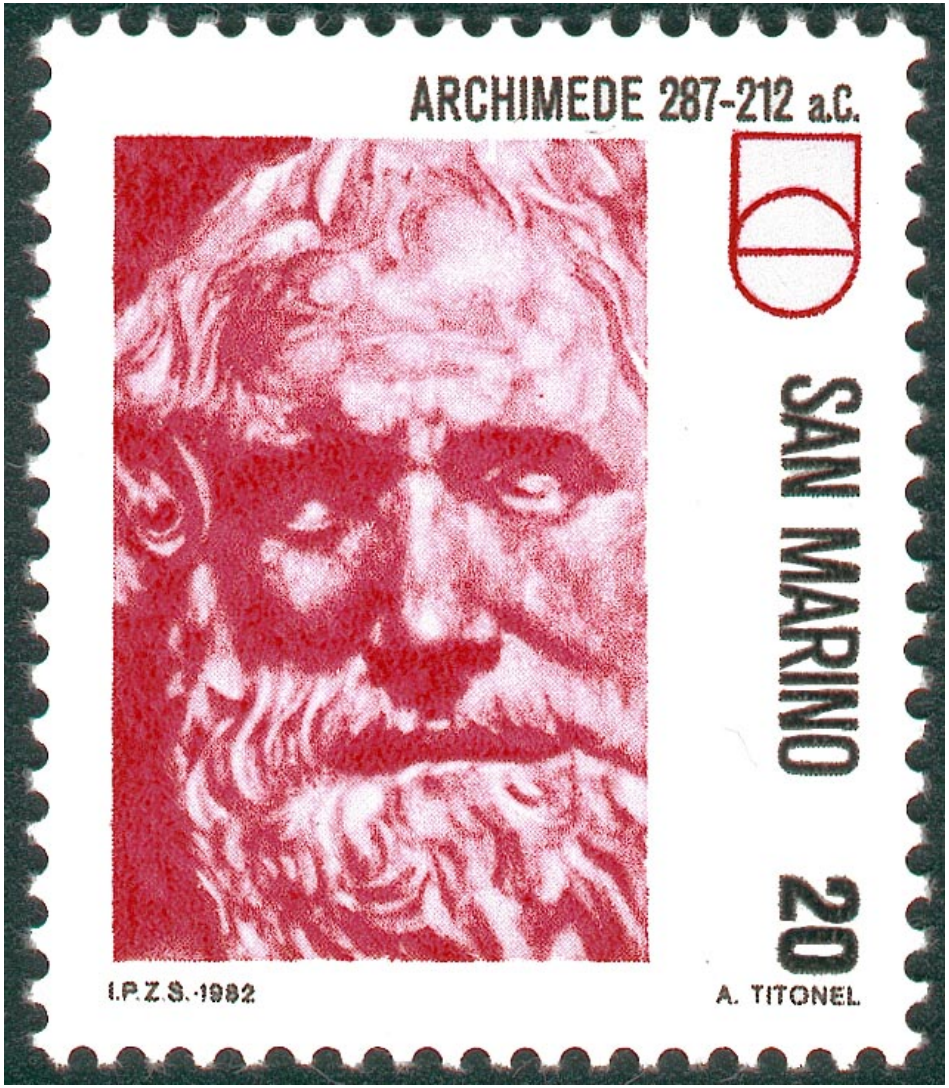
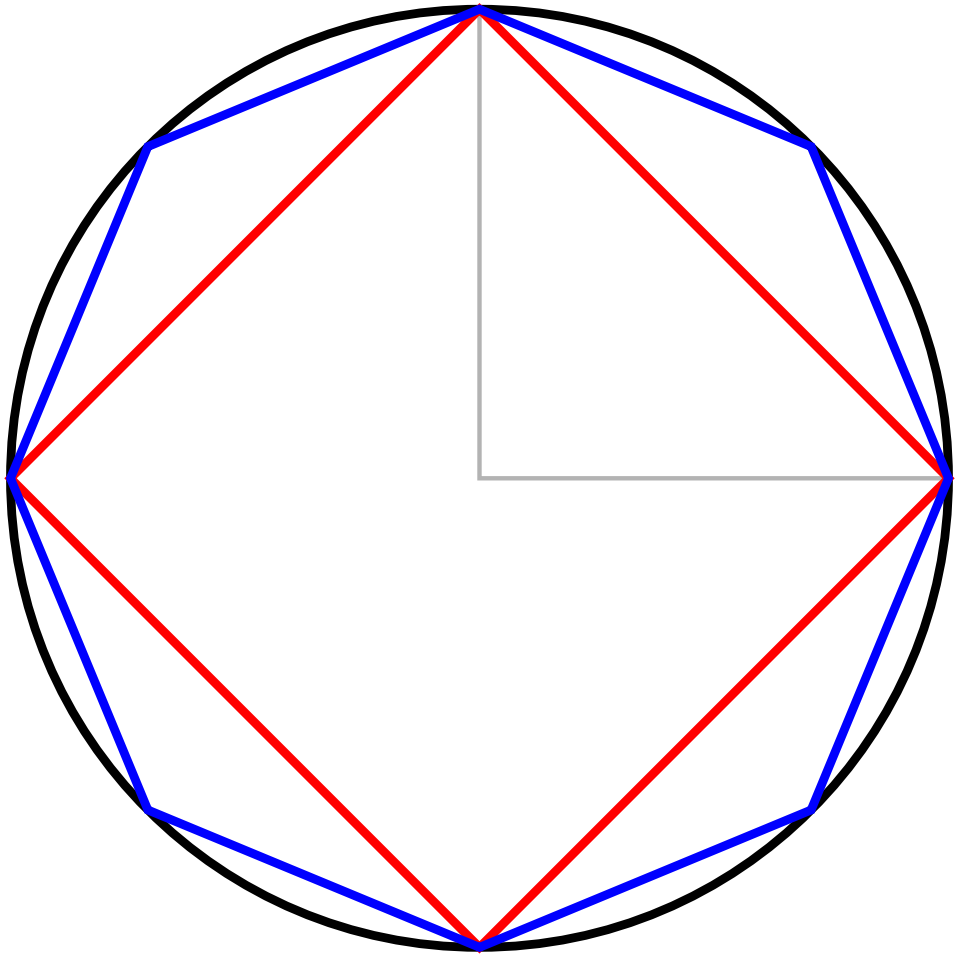
What's π to ten digits?

If you couldn't look it up, how would you figure it out?

Archimedes method

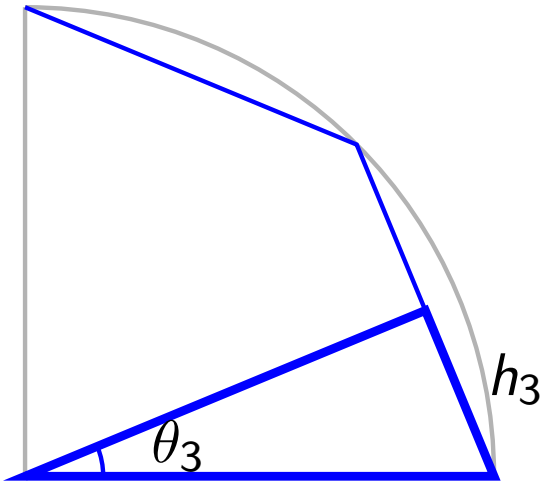


Archimedes method



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

$$\begin{aligned}\sin^2(\theta_k) &= 4\sin^2(\theta_{k+1})\cos^2(\theta_{k+1}) \\ &= 4\left(\sin^2(\theta_{k+1}) - \sin^4(\theta_{k+1})\right)\end{aligned}$$

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

$$z^2 - z + h_k^2/4 = 0.$$

We know the quadratic formula, right?

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

Computing π, take 1

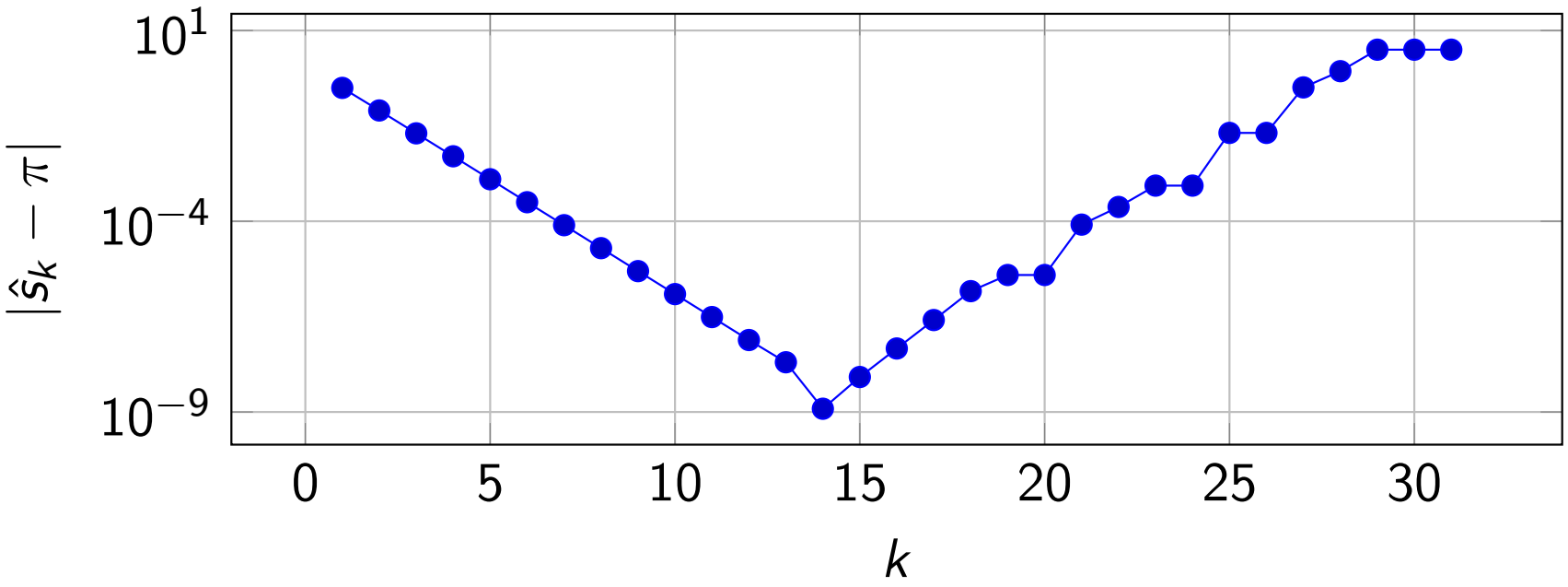
Compute half-side-lengths by recurrence:

$$h_2^2 = 1/2$$
$$h_{k+1}^2 = \frac{1}{2}\left(1 - \sqrt{1 - h_k^2}\right)$$

Then use

$$\pi \approx 2^k h_k$$

Uh-oh



At $k = 30$, computer claim $s_k = 0$!

Computing π, take 2

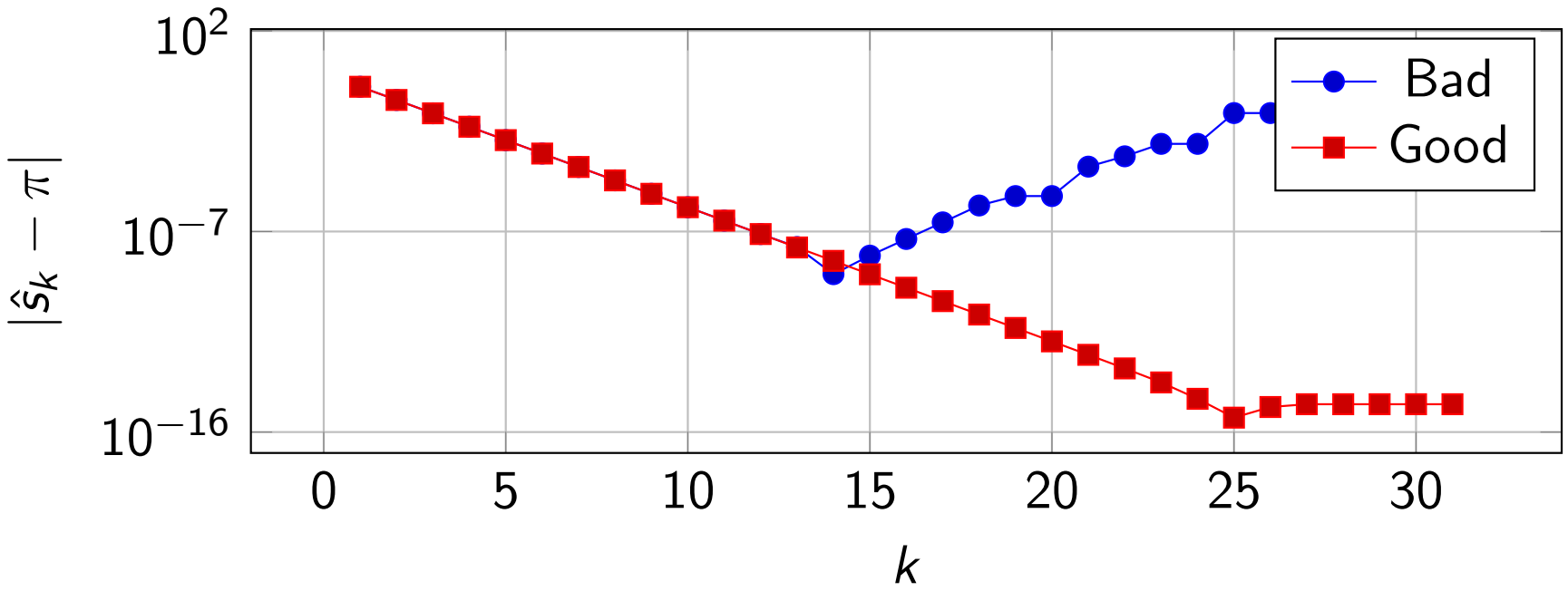
Problematic formula:

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

We know how to fix this!

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

Better



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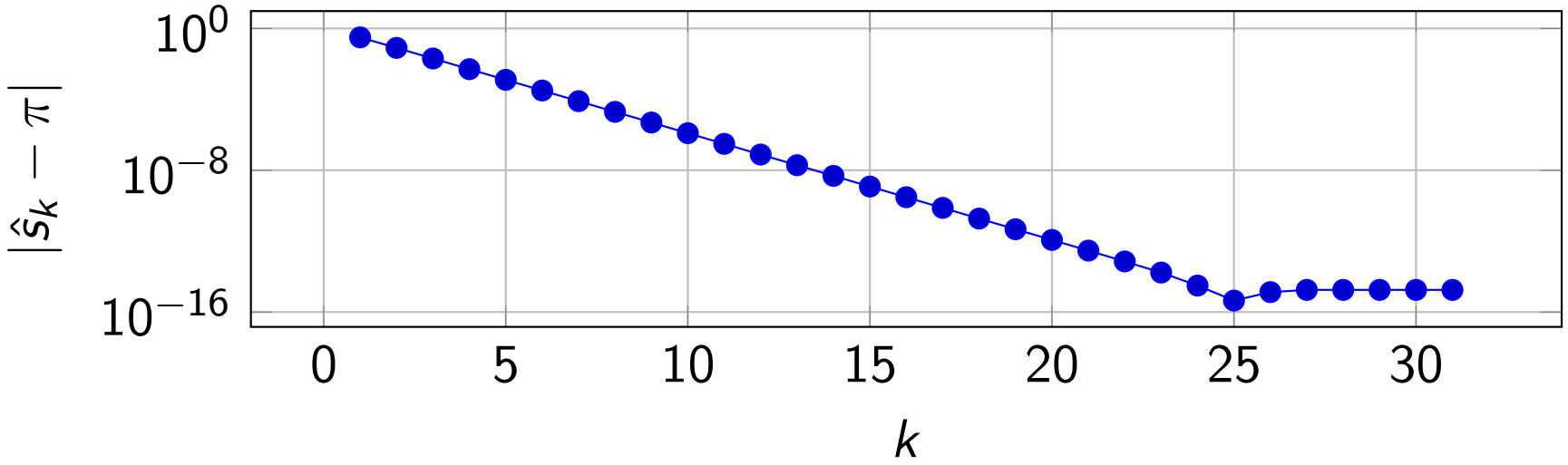
Model Madness

Hmm



Convergence looks *very* systematic. In fact

$$2^k h_k = 2^k \left(2^{-k}\pi - \frac{1}{6}(2^{-k}\pi)^3 + \dots \right)$$
$$= \pi - \frac{\pi^3}{6} 2^{-2k} + O(2^{-4k})$$

The error at step k is about four times the error at step $k+1$.

Extrapolation / Acceleration

If e_k is the error at step k, then

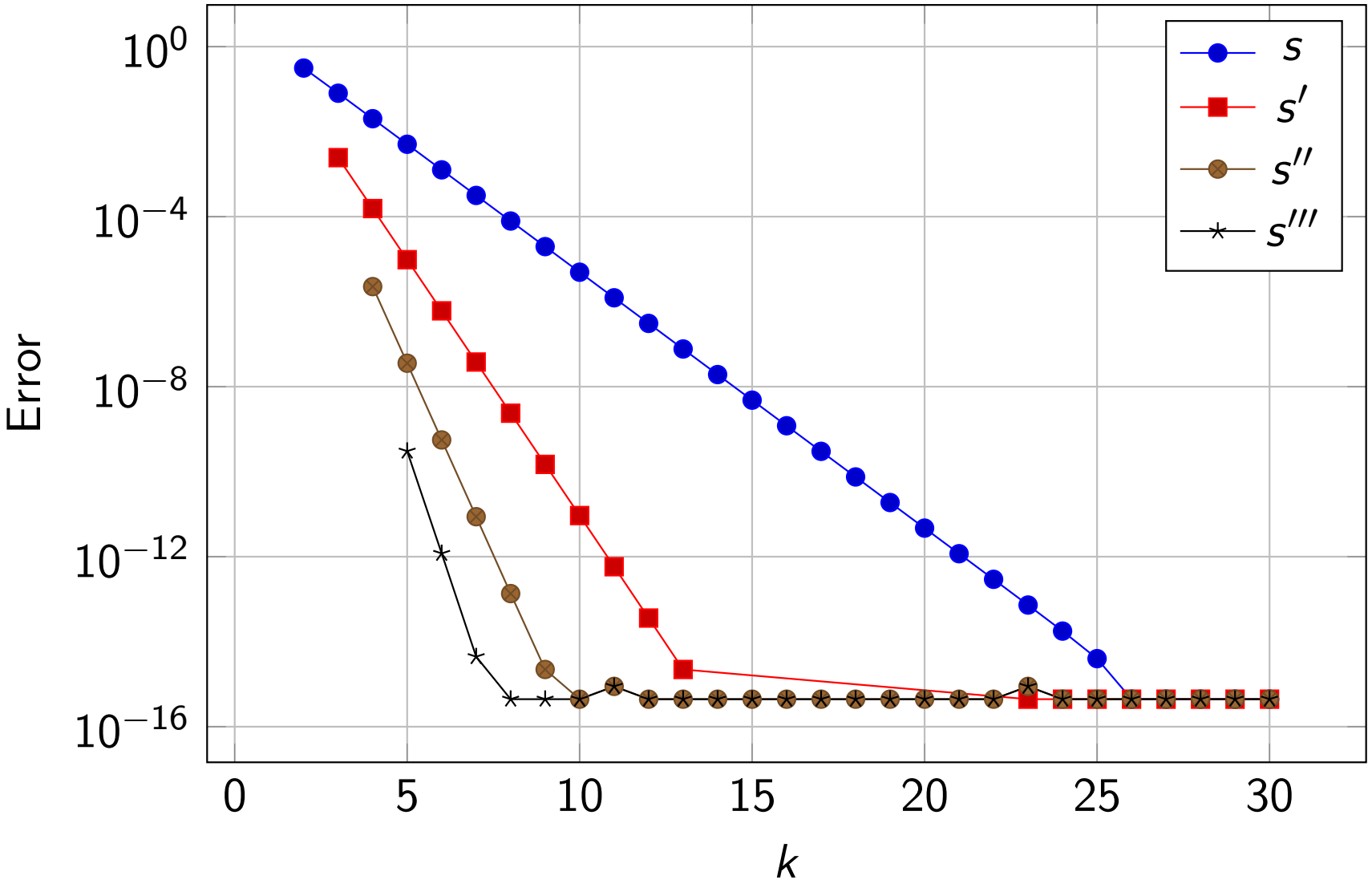
$$s_k = \pi + e_k$$
$$s_{k+1} = \pi + e_k/4 + \epsilon$$

Combine:

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

Rinse, wash, repeat!

Accelerated Convergence



Another Approach

Another formula for π:

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

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 $e_k \approx \alpha q^k$.

$$\begin{aligned} s_{k-1} &\approx A + \alpha q^{k-1} \\ s_k &\approx A + \alpha q^k \\ s_{k+1} &\approx A + \alpha q^{k+1} \end{aligned}$$

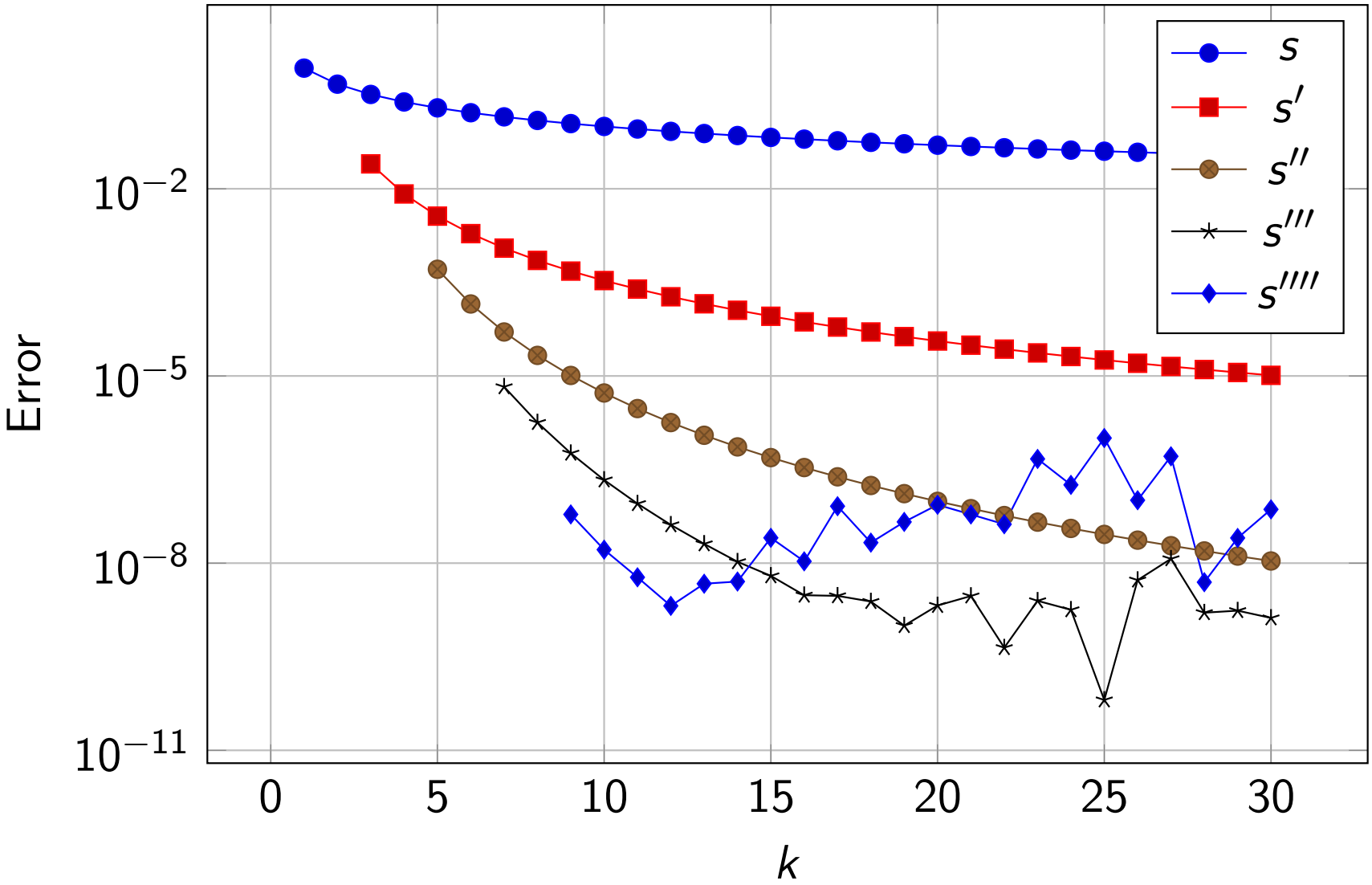
Have

$$q \approx \frac{s_{k+1} - s_k}{s_k - s_{k-1}}, \qquad A \approx \frac{q^{-1} s_{k+1} - s_k}{q^{-1} - 1}$$

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



Full circle

- 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.