The Theodorus Spiral: An Exercise in Functional Equations, Summation of Series, Quadrature, and Asymptotics

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Swiss Numerical-Analysis Colloquium
University of Basel, April 24, 2009

Abstract

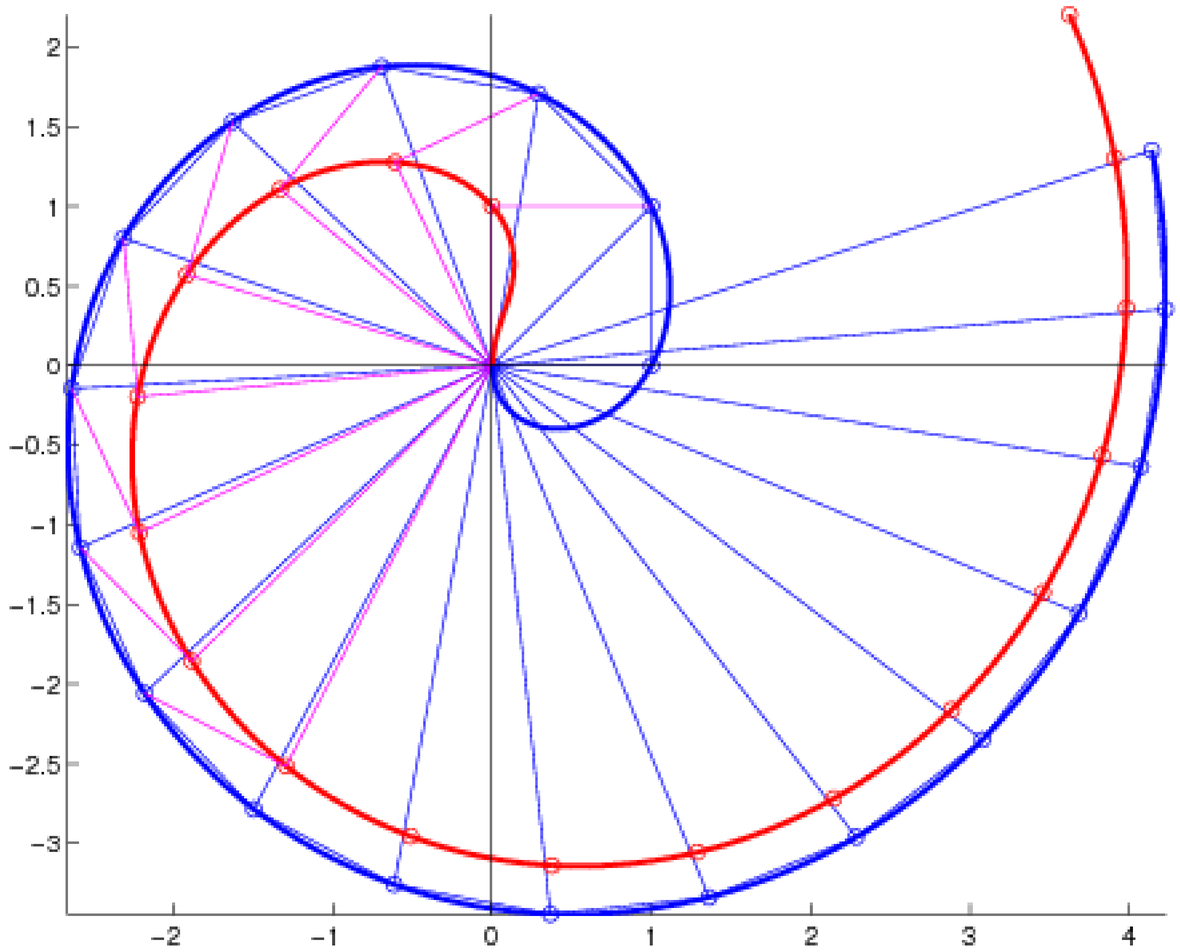
The remarkable classical pattern of the discrete Theodorus spiral, or square root spiral, can intuitively be supplemented by a closely related inner spiral asymptotic to it. A "nice" interpolating analytic curve was constructed by Philip J. Davis (1993) as an infinite product satisfying the same functional equation as the discrete points. The analytic continuation of the Davis solution to a different sheet of its Riemann surface interpolates the points of both spirals.

References

Philip J. Davis: Spirals: From Theodorus to Chaos. A. K. Peters, 1993, 220 pp.

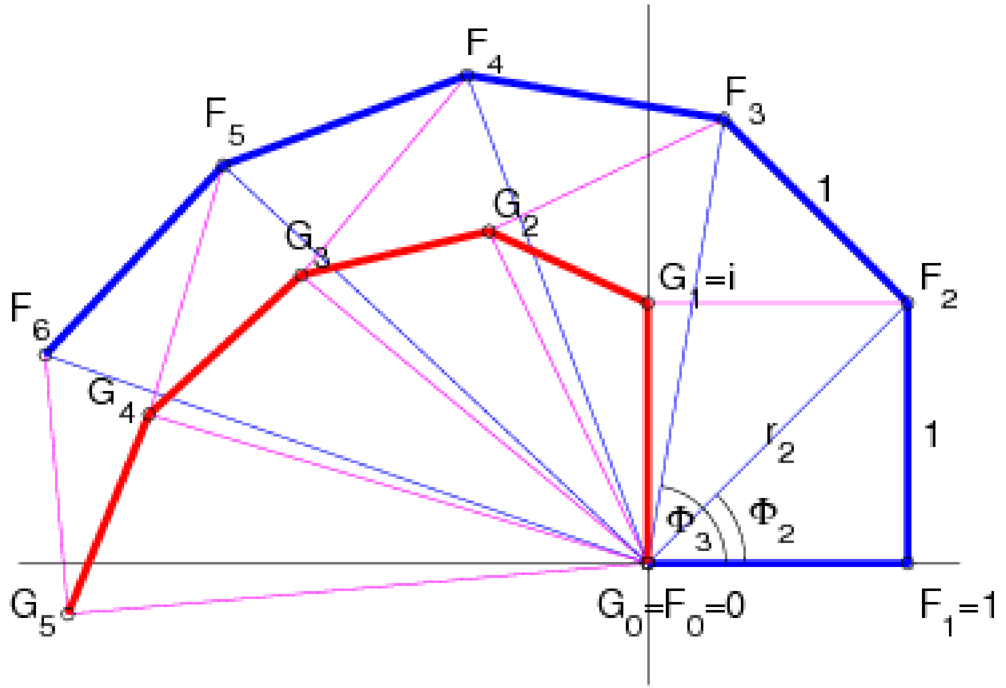
Walter Gautschi: The spiral of Theodorus, special functions, and numerical analysis. In Ph.J. Davis, loc. cit., 67-87.

The Twin Spiral and its Common Monotonic Analytic Interpolant



Outline

1. A Functional Equation



The outer discrete spiral, complex coordinates and polar coordinates:

$$F_n = r_n \, e^{i\,\Phi_n}\,, \quad r_n = |F_n|\,, \quad \Phi_n = \arg F_n\,, \quad n = 1, 2, \dots\,, \qquad (1)$$

Relations (functional equation):

$$r_n = \sqrt{n}\,, \quad \Phi_{n+1} - \Phi_n = \arctan\left(\frac{1}{\sqrt{n}}\right), \quad \Phi_1 = 0\,, \quad n \in \mathbb{N}\,. \tag{2}$$

Cumulative sum and product for $n \in \mathbb{N}$:

$$\Phi_n = \sum_{k=1}^{n-1} \arctan\left(\frac{1}{\sqrt{k}}\right), \quad F_n = \prod_{k=1}^{n-1}\left(1 + \frac{i}{\sqrt{k}}\right), \quad n \in \mathbb{N}\,. \tag{3}$$

The inner discrete spiral G_n is obtained from

$$G_n \cdot \left(1 - \frac{i}{r_n}\right) = F_{n+1} = F_n \cdot \left(1 + \frac{i}{r_n}\right), \quad r_n = \sqrt{n}\,, \quad F_1 = 1\,. \tag{4}$$

Ph. J. Davis' Interpolating Curve, 1993

Use Euler's idea of "telescoping" infinite products (or sums) for constructing the gamma function as an interpolant to the factorial:

$$\Phi_n = \sum_{k=1}^{\infty} \left\{ \arctan\left(\frac{1}{\sqrt{k}}\right) - \arctan\left(\frac{1}{\sqrt{k-1+n}}\right) \right\} . \qquad (5)$$

Given also in the reference Heuvers, Moak, Boursaw (HMB), 2000 (Slide13)

For $n \in \mathbb{N}$ this is equivalent with the finite sum (3), therefore satisfies the functional equation (2). The infinte sum converges absolutely for $n \in \mathbb{R}_+$; therefore (5) defines an analytic solution of (2).

Substituting (5) into (1) yields Davis' infinite product

$$F_n = F(n) = \prod_{k=1}^{\infty} \frac{1 + \dfrac{i}{\sqrt{k}}}{1 + \dfrac{i}{\sqrt{k-1+n}}} , \quad n \in \mathbb{R}_+ . \qquad (6)$$

2. Analytic Continuation

A natural new parameter: $r := \pm\sqrt{n} \in \mathbb{R}, \quad \Phi_n = \Phi(n) = \Phi(r^2) =: \varphi(r)$

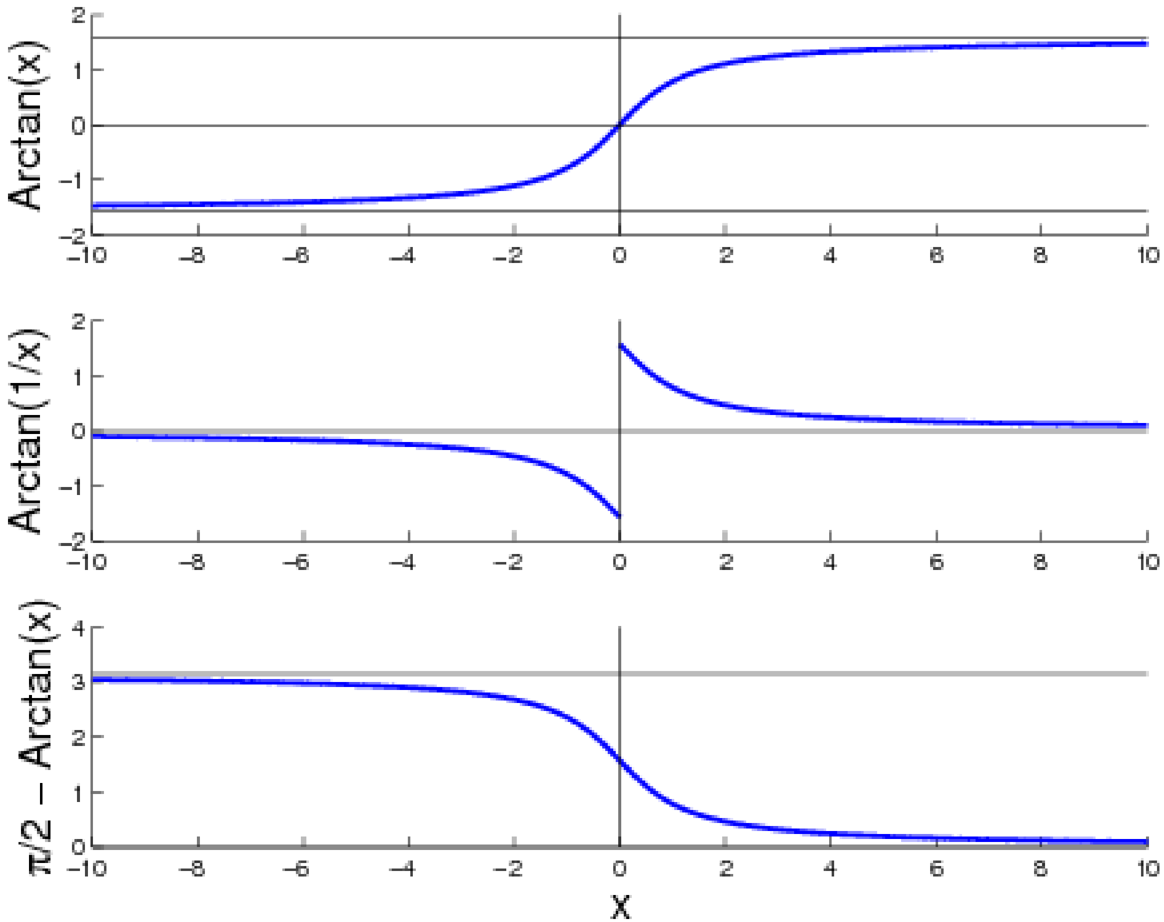
In the terms T_k of (5) with $k > 1$ all square roots must consistently be taken with the positive sign for any value of $n = r^2$. In contrast, the term T_1 with $k = 1$ passes through a branch point at $r = 0$. The analytic continuation of T_1 to negative values of r changes the sheet of its Riemann surface at $r = 0$.

Analytic continuation:

$$\arctan\left(\frac{1}{r}\right) = \frac{\pi}{2} - \operatorname{Arctan}(r)\,, \;\; r \in \mathbb{R}\,. \tag{7}$$

$\operatorname{Arctan}(r)$ denotes the principal branch of the arctan function with branch cuts on the imaginary axis from i to $i\,\infty$ and from $-i\,\infty$ to $-i$.

The arctan Function



Equation (5) with $n = r^2,\ r \in \mathbb{R}$ becomes

$$\varphi(r) = -\frac{\pi}{4} + \mathrm{Arctan}(r) + \sum_{k=2}^{\infty} \left\{ \arctan\left(\frac{1}{\sqrt{k}}\right) - \arctan\left(\frac{1}{\sqrt{k-1+r^2}}\right) \right\} . \tag{8}$$

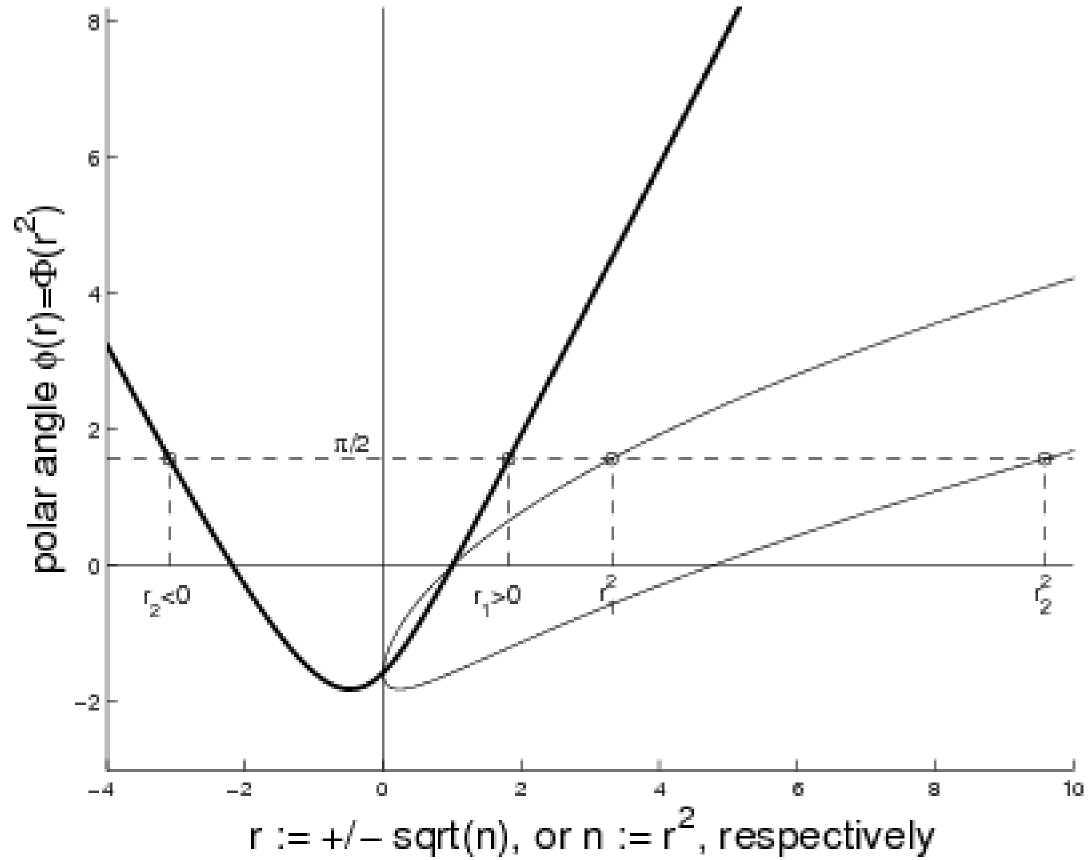
$\varphi(r)$ satisfies the functional equation

$$\varphi(\sqrt{r^2+1}) = \varphi(r) + \frac{\pi}{2} - \mathrm{Arctan}(r)\,, \quad r \in \mathbb{R}\,, \tag{9}$$

and the sign change in r is governed by

$$\varphi(-r) = \varphi(r) - 2\,\mathrm{Arctan}(r)\,, \quad r \in \mathbb{R}\,. \tag{10}$$

The Functions $\varphi(r)$ and $\Phi(r^2)$



The polar angle $\varphi(r) = \Phi(r^2)$ as a function of r or of r^2. The marked points are $r_1 = 1.8191988282,\ r_2 = -3.0958799878,\ \varphi = \Phi = \pi/2$

3. Uniqueness

A functional equation of the type of p. 6, Equ. (2) has many "nice", even analytic, solutions.

Example:

$$F(x+1) - F(x) = 1 \quad \text{is solved by} \quad F(x) = x + p(x)\,,$$

where p is any 1-periodic function, e.g. $p(x) = c\,\sin(2\,\pi\,x)$.

Distinguished solution: No oscillations, monotonic derivative $\Longrightarrow$

$$p(x) = \text{const.}\,, \quad F(x) = x + \text{const.}\,.$$

Monotonic F is unique up to a constant.

Theorem by HMB and Gronau

General solution of the functional equation (2): $\Psi(n) = p(n) + \Phi(n)$ with $p(n)$ being any 1-periodic function, and $\Phi(n)$ is defined in Equ. (5). If $\Psi(n)$ is monotonically increasing, $p(n)$ is a constant function. If in addition $\Psi(1) = 0$ then $p(n) = 0$.

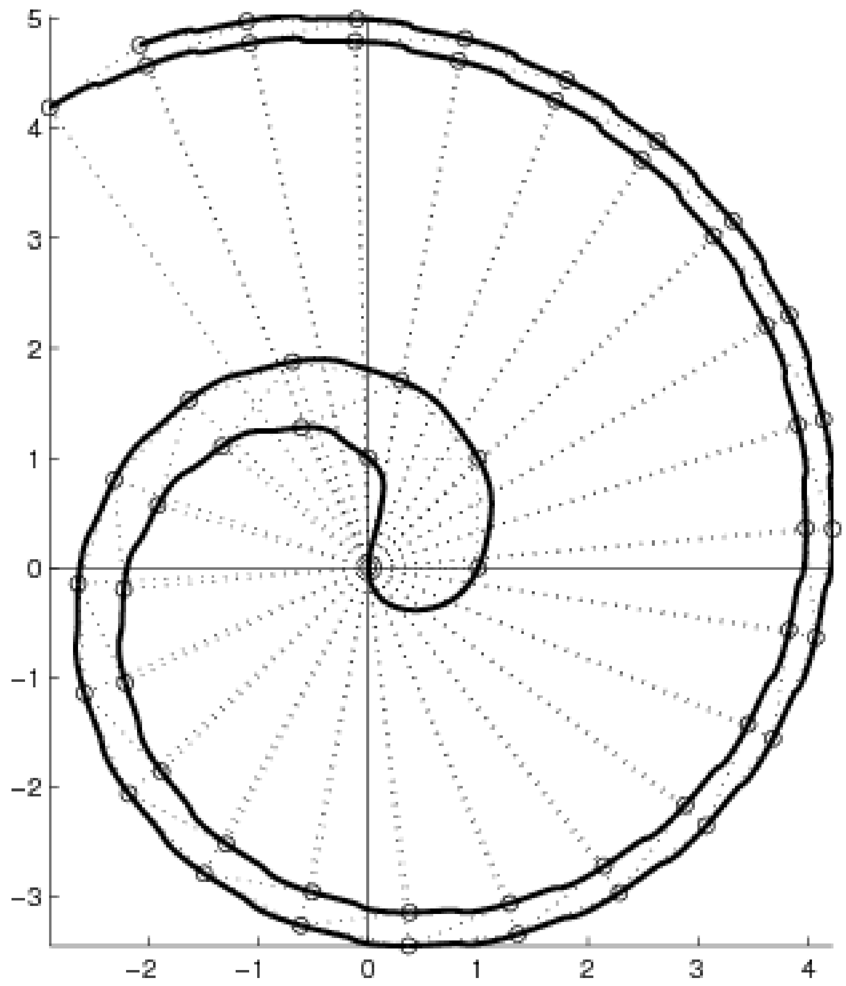
References

K.J. Heuvers, D.S. Moak and B. Boursaw: The functional equation of the square root spiral. In: T.M. Rassias (ed.): Functional Equations and Inequalities, Kluver, 2000, 111-117.

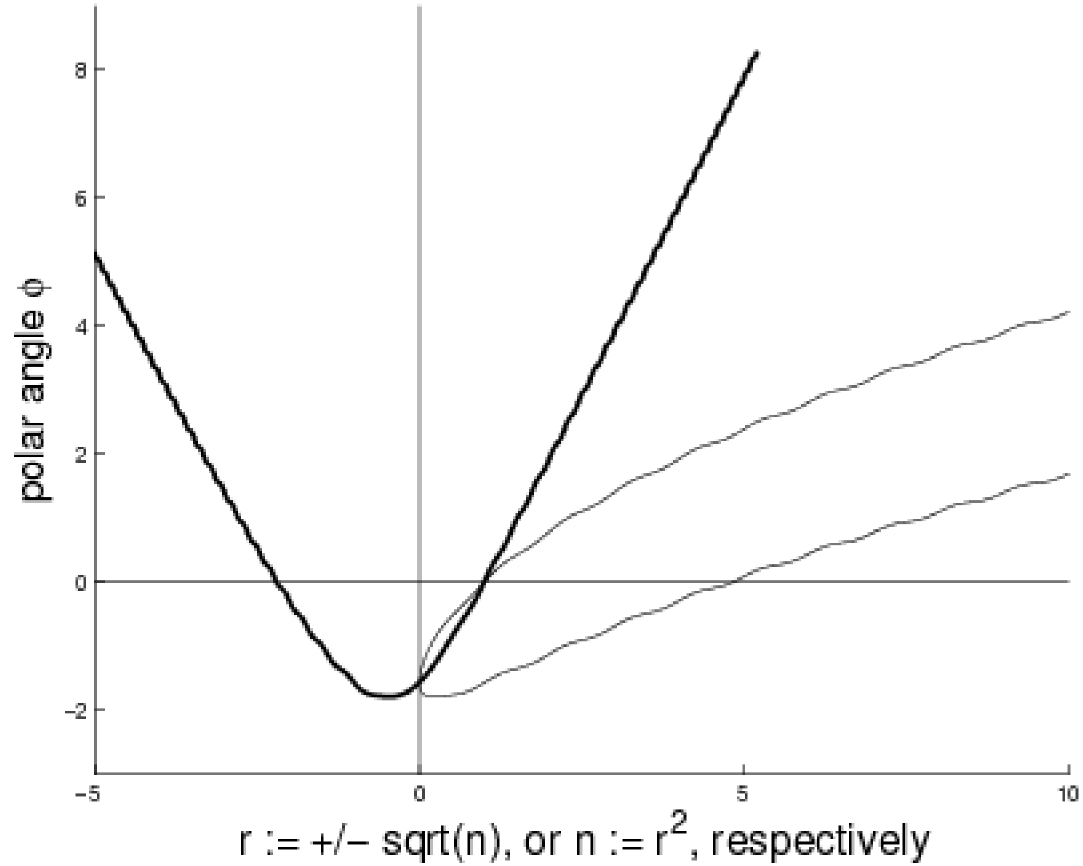
Detlef Gronau: The spiral of Theodorus. Amer. Math. Monthly **111**, 2004, 230-237.

Steven Finch: Constant of Theodorus. http://algo.inria.fr/csolve/th.pdf, April 9, 2005.

A Non-Monotonic Spiral



Corresponding Non-Monotonic Polar Angle



Polar angle: $\Phi_{\mathrm{nonmon}}(r^2) = \Phi(r^2) + 0.03\,\sin(2\,\pi\,r^2)$

4. Summation of Series by Contour Integration

Efficient evaluation of (8). $r \in [0, 1]$ suffices; otherwise use (9), (10).

- Difficulty: Slowly converging series.
- Helpful: Terms depend analytically on the index k.
- Techniques of accelerating convergence may help a little bit.

  There are better methods:

- Write the sum as a contour integral (Residue theorem backwards).
- Deform the path of integration appropriately.
- Trapezoidal rule (after appropriate transformation of the integrand).

A Summation Formula

The function $z \mapsto \pi \, \mathrm{cotan}(\pi \, z)$ has a first-order pole of residue 1 at every integer point. Use a contour C passing from ∞ in the first quadrant to ∞ in the fourth quadrant, intersecting the real line in the interval $(0, 1)$. Deform C into the line $z = \frac{1}{2} + i\, y$, $\infty > y > -\infty$. This yields the

Theorem: Let $s : z \mapsto s(z)$ be analytic in $D := \{z \,\big|\, |\arg(z)| < \pi/2\}$ with $s(\bar{z}) = \overline{s(z)}$ and $s(z) = O(z^{-\alpha})$, $\alpha > 1$ as $|z| \to \infty$, $z \in D$. Then

$$S := \sum_{k=1}^{\infty} s(k) = \frac{1}{2} \int_{-\infty}^{\infty} \mathrm{Im}\, s(\frac{1}{2} - i\, y) \;\tanh(\pi\, y)\; dy\,. \qquad \Box$$

Application to the Sum in Equ. (8)

To avoid cancellation, write the term $\{\ldots\}$ in the sum (8) as

$$s(z) := \arctan\left(\frac{r^2-1}{(z+r^2)\sqrt{z}+(z+1)\sqrt{z+r^2-1}}\right).$$

In view of (8) use the contour

$$z = \frac{3}{2} - i\,y\,.$$

The change of variables

$$y = \sinh\big(\sinh(t)\big), \quad dy = \cosh\big(\sinh(t)\big)\,\cosh(t)\,dt, \quad t \in \mathbb{R}$$

yields a quickly decaying integrand (doubly exponential decay).

5. Transformations

Use an appropriate transformation $x = \phi(t)$, $t \in \mathbb{R}$ in order to transform the integral under consideration,

$$I = \int_a^b f(x)\,dx\,,$$

to the integral of a quickly decaying analytic function over $\mathbb{R}$.

Desired properties of ϕ:

- analytic, monotonic
- quickly and accurately computable, e.g. a combination of elementary functions

Result:

$$I = \int_{-\infty}^{\infty} g(t)\,dt \quad \text{with} \quad g(t) := f\big(\phi(t)\big)\,\phi'(t)$$

Examples

Interval	Transformation
1. Finite interval, $x \in (-1, 1)$:	$x = \phi_1(t) = \tanh(t/2)$
2. Finite interval, $x \in (0, 1)$:	$x = \phi_2(t) = \dfrac{1}{1 + \exp(-t)}$
3. Semi-infinite interval, $x \in (0, \infty)$:	$x = \phi_3(t) = \exp(t)$
4. Real line $\mathbb{R}$, enhance the decay:	$x = \phi_4(t) = \sinh(t)$
5. Real line $\mathbb{R}$, enhance decay as $t \to +\infty$:	$x = \phi_5(t) = t + \exp(t)$
6. Real line $\mathbb{R}$, enhance decay as $t \to -\infty$:	$x = \phi_6(t) = t - \exp(-t)$

Remark. In the case of finite boundaries integrable boundary singularities are allowed.

6. Numerical Quadrature by the Trapezoidal Rule

Let f be such that its integral over $\mathbb{R}$ exists,

$$I = \int_{-\infty}^{\infty} f(x)\, dx.$$

Trapezoidal sum, step h, offset τ :

$$T(h,\tau) = h \sum_{j=-\infty}^{\infty} f(\tau + j\, h),$$

Periodicity:

$$T(h,\tau) = T(h,\tau + h)$$

Refinement:

$$T(\frac{h}{2},\tau) = \frac{1}{2}\left(T(h,\tau) + T(h,\tau + \frac{h}{2})\right)$$

Truncation of Infinite Trapezoidal Sums

$$\tilde{T}(h,s) = h \sum_{j=n_0}^{n_1} f(s+jh).$$

Desirable truncation rule: Truncate if $|f(x)| < \varepsilon$, where $x := s + jh$, and $\varepsilon > 0$ is a given tolerance reflecting the working precision.

A (moderately) robust implementation:

- Choose an interior point x_0 and accumulate two separate sums upwards from $x_0 + h$ and downwards from x_0
- Truncate each sum if two (or three) consecutive terms do not contribute to the sum

The Truncation Error

Remainder for the truncation limit X:

$$R_X := \int_X^\infty f(x)\,dx, \quad \text{where} \quad f(X) = \varepsilon$$

(i) Algebraic decay:

$$f(x) = x^{-\alpha-1}, \quad (\alpha > 0), \qquad R_X = \frac{X^{-\alpha}}{\alpha} = \frac{\varepsilon^{\alpha/(1+\alpha)}}{\alpha}$$

No good! Remainder may be $>> \varepsilon$. E. g. $R_X = O(\sqrt{\varepsilon})$ for $\alpha = 1$.

(ii) Exponential decay:

$$f(x) = e^{-\alpha x}, \quad (\alpha > 0), \qquad R_X = \frac{1}{\alpha}\,e^{-\alpha X} = \frac{\varepsilon}{\alpha}$$

Better, but dangerous if $\alpha << 1$.

(iii) Doubly exponential decay:

$$\begin{aligned} f(x) &= \exp(-e^{\alpha\, x}), \quad (\alpha > 0), \\ R_X &= \frac{1}{\alpha}\, \exp(-e^{\alpha\, X})\, \left(e^{-\alpha\, X} - e^{-2\,\alpha\, X} + 2!\, e^{-3\,\alpha\, X} + \ldots\right) \end{aligned}$$

Truncation limit:

$$f(X) = \varepsilon \implies X = \frac{1}{\alpha}\, \log\log\frac{1}{\varepsilon}\ ,$$

therefore

$$R_X = -\frac{\varepsilon}{\alpha}\left(\frac{1}{\log\, \varepsilon} + O((\log\, \varepsilon)^{-2})\right).$$

Truncation is safe even for $\alpha << 1$ if ε is sufficiently small.

The Discretization Error

$$I = \int_{-\infty}^{\infty} f(x)\, dx.$$

Fourier Transform: $\hat{f}(\omega) := \int_{-\infty}^{\infty} e^{-i\,\omega\,x}\ f(x)\ dx\,, \quad I = \hat{f}(0)$

Trapezoidal sum with offset: $T(h,\tau) := h\ \sum_{j=-\infty}^{\infty} f(j\,h + \tau)$

Poisson summation formula: $T(h,\tau) = PV \sum_{k=-\infty}^{\infty} \hat{f}\left(k\,\frac{2\pi}{h}\right)\ e^{i\,\tau\,k\cdot 2\pi/h}$

For offset $\tau = 0$ we obtain the error formula

$$T(h,0) - I = \hat{f}\left(\frac{2\pi}{h}\right) + \hat{f}\left(-\frac{2\pi}{h}\right) + \hat{f}\left(\frac{4\pi}{h}\right) + \hat{f}\left(-\frac{4\pi}{h}\right) + \ldots$$

Theorem. The discretization error of the infinite trapezoidal sum for a small step $h > 0$ is asymptotic to the sum of the Fourier transform values of the integrand at $\pm 2\pi/h$.

Particular cases

(i) Integrand analytic in a strip of the complex plane

Let $f(x)$ be analytic in $\left|\mathrm{Im}(x)\right| < \gamma,\ \gamma > 0$. Then

$$\left|\hat{f}(\omega)\right| = O(e^{-(\gamma-\varepsilon)\,|\omega|}) \quad \text{for any} \quad \varepsilon > 0, \quad \text{as} \quad \omega \to \pm\infty\,,$$

and the discretization error for $h \to 0$ is

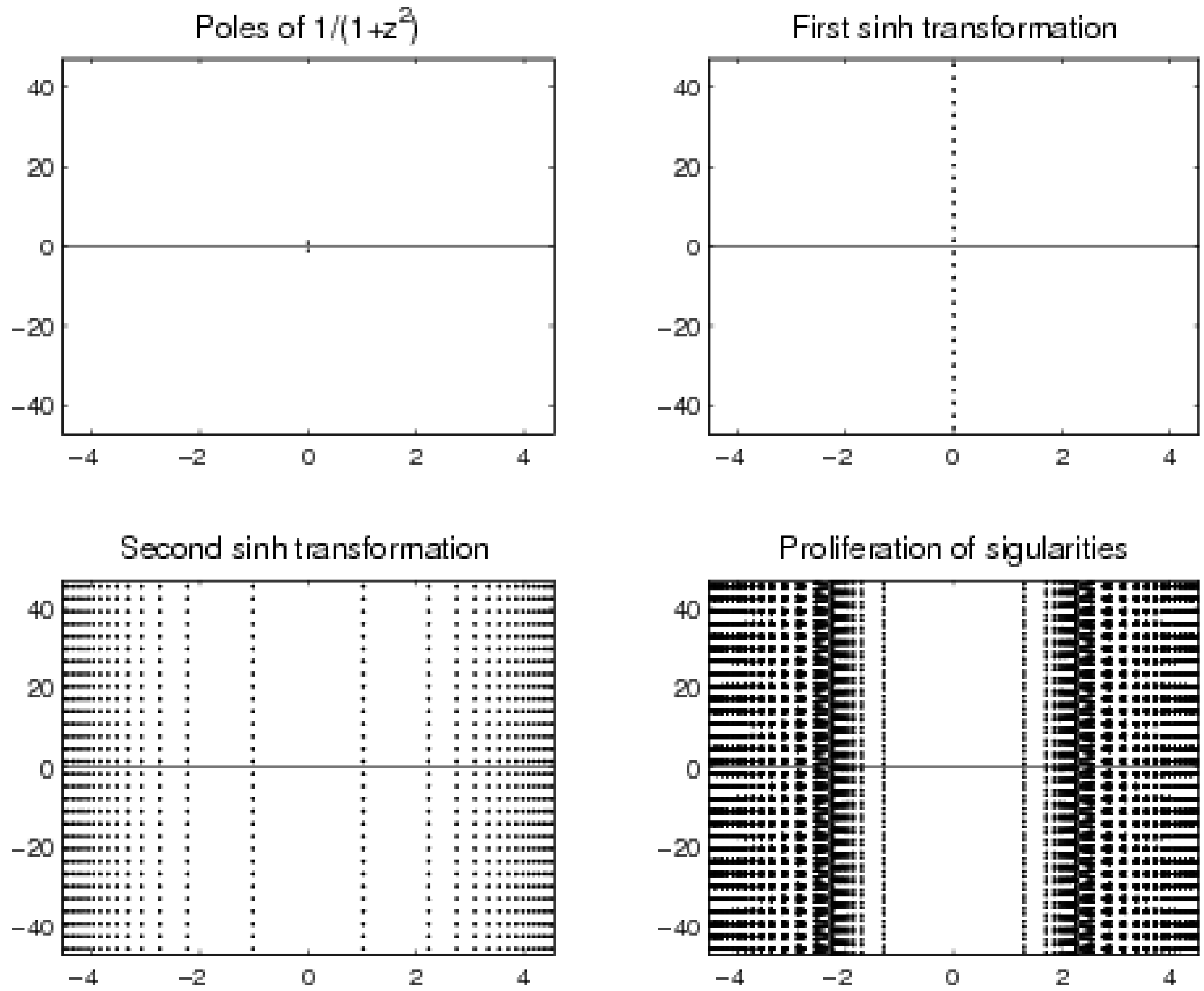
$$T(h,0) - I = O(e^{-(\gamma-\varepsilon)\,\omega}) \quad \text{with} \quad \omega := 2\,\pi/h.$$

(ii) Proliferation of singularities due to sinh transformations

Convergence may be slower, such as (with some $\gamma > 0$)

$$T(h,0) - I = O(e^{-\gamma\,\omega/\log(\omega)}) \quad \text{or} \quad T(h,0) - I = O(e^{-\gamma\,\sqrt{\omega}}).$$

Breeding Singularities by sinh Transformations, $\int_{-\infty}^{\infty} \frac{dz}{1+z^2}$



Experiments in PARI/GP

Evaluating the sum in (8) by means of the PARI function

```
{fct(t) =
  sh = sinh(t); y = sinh(sh); dy = cosh(sh)*cosh(t); z = 3/2 + I*y;
  dy * tanh(Pi*y) * imag(atan((1-rr)/((z+rr)*sqrt(z)+(z+1)*sqrt(z+rr-1))))
}
```

with the global argument rr$=r^2 = 0.25$ and the trapezoidal rule with steps $h = 1, \frac{1}{2}, \frac{1}{4}, \ldots$ yields (with a loss of at most 2 digits):

Working precision	19	38	67	105	144	192	298	404
Reciprocal step	32	64	128	256	512	512	1024	2048
1.6 GHz seconds	.015	.05	.19	.70	2.35	4.04	18.6	67.9

C. Batut, K. Belabas, D. Bernardi, H. Cohen, M. Olivier:
The software package PARI. http://pari.math.u-bordeaux.fr/

7. Asymptotics

Equation (2) admits a formal solution of the form

$$\Phi(n) = \gamma(n) + c_0\, n^{1/2} + c_1\, n^{-1/2} + c_2\, n^{-3/2} + \ldots, \qquad (11)$$

where $\gamma(n)$ is any 1-periodic function of n. The coefficients c_k satisfy the relation

$$\sum_{l=0}^{k} \binom{\frac{1}{2}-l}{k+1-l} c_l = \frac{(-1)^k}{2\,k+1}, \quad k = 0, 1, 2, \ldots, \qquad (12)$$

which may be solved recursively by

$$c_k = \frac{2\,(-1)^k}{1-4\,k^2} - \sum_{l=0}^{k-1} \binom{\frac{1}{2}-l}{k-l} \frac{c_l}{k+1-l}, \quad k = 0, 1, 2, \ldots. \qquad (13)$$

The first few coefficients are found to be

$$c_0 = 2,\ c_1 = \frac{1}{6},\ c_2 = -\frac{1}{120},\ c_3 = -\frac{1}{840},\ c_4 = \frac{5}{8064},\ c_5 = \frac{1}{4224},\ c_6 = -\frac{521}{2196480}.$$

- Coefficients seem to decrease
- The numerator 521 destroys any hope for a simple behaviour
- $\gamma(n) = \gamma =$ const. yields "distinguished" solutions, monotonic at ∞
- Comparison of (11) with the sum (3) yields (n=52, 36 terms in (11))

$$\gamma = -2.15778\,29966\,59446\,22092\,91427\,86829\,57772\,35041\,39598\,60756$$

- Unfortunately, this is not rigorous since the series (11) is divergent

The Series Coefficients

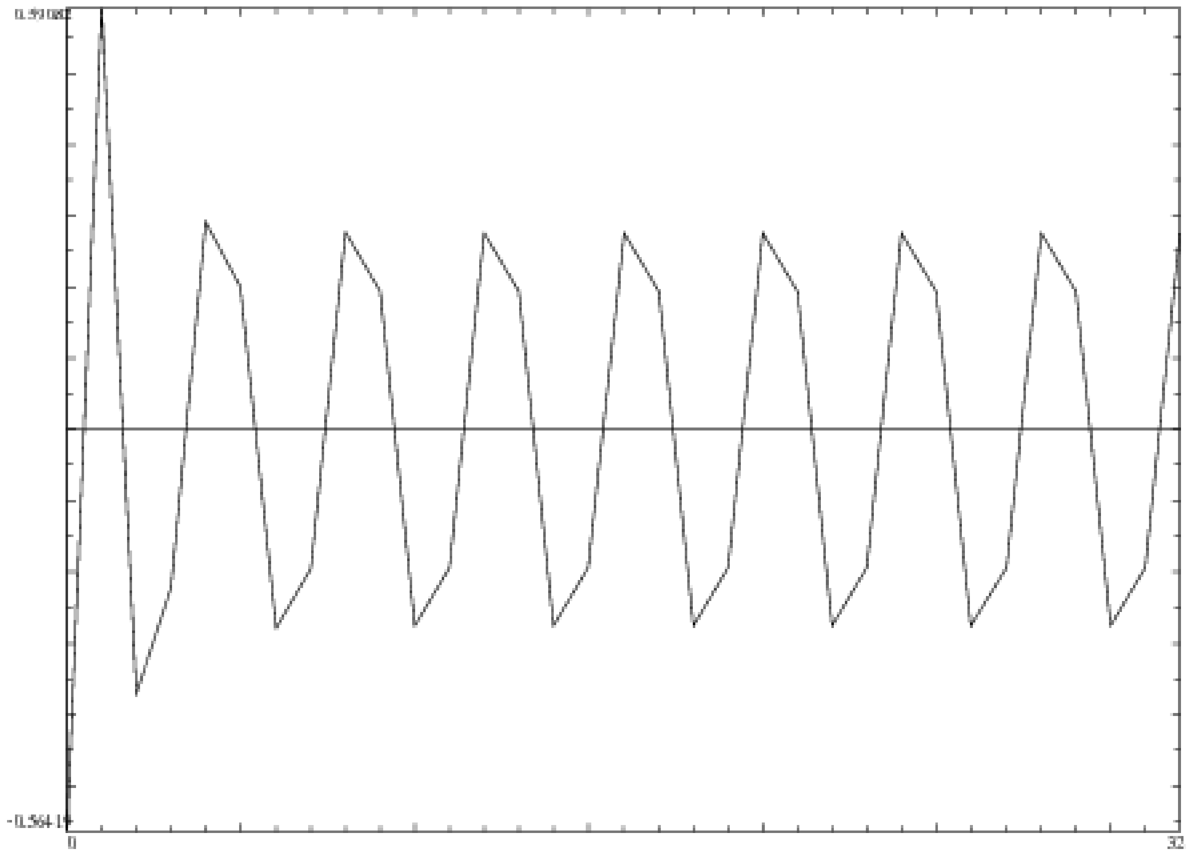
Equ. (12) may be written by means of a lower triangular matrix L and a column vector $\mathbf{c} = [c_0, c_1, \ldots]^T$. The inverse matrix (also lower triangular) is given by

$$L^{-1} = \Big(m_{kl}\Big)\,, \quad m_{kl} = (-1)^{k+1-l}\,\frac{B_{k-l}}{k-\frac{1}{2}}\binom{k-\frac{1}{2}}{k-l}\,, \quad l \le k\,,$$

where B_j are the Bernoulli numbers. This leads to a closed form of the coefficients c_l, resulting in the asymptotic formula (for $l \to \infty$)

$$c_l \sim \frac{(l-\frac{3}{2})!}{(2\,\pi)^l}\,\mathrm{Re}(\rho\, i^{\,l})\,, \quad \rho = .27547 - .19375\, i = \frac{\mathrm{erf}(z)}{z}\,,\ z = \sqrt{\pi}\,(1+i)\,.$$

Coefficients of the Asymptotic Series, Scaled



Scaled coefficients, $c_l\,(2\,\pi)^l\,(l-\frac{3}{2})!$, versus $l \le 32$

The Euler Constant of the Theodorus Spiral (Slide 30)

$$\gamma = \lim_{n\to\infty} \sum_{k=1}^{n-1} \left(\arctan\left(\frac{1}{\sqrt{k}}\right) - 2\sqrt{n} \right) = -2.15778\,29966\,59446\ldots$$

Use the Euler-Maclarin summation formula with remainder term:

$$\sum_{k=1'}^{n'} f(k) = \int_1^n f(x)\,dx - f(n) + \int_1^n \left(\{x\} - \frac{1}{2}\right) f'(x)\,dx\,.$$

With $f(x) := \arctan\left(x^{-1/2}\right)$ we obtain

$$\gamma = -\frac{3}{8}\pi - 1 + \sum_{m=1}^{\infty} g(m)\,,$$

where

$$\begin{aligned} g(m) \quad &:= \quad (m+\tfrac{3}{2})\arctan\left(\frac{1}{(m+2)\sqrt{m} + (m+1)^{3/2}}\right) - \frac{1}{\sqrt{m+1}+\sqrt{m}} \\ &= \quad \frac{1}{16}m^{-5/2} - \frac{35}{192}m^{-7/2} + \frac{105}{256}m^{-9/2} - \frac{27}{32}m^{-9/2} + O\left(m^{-13/2}\right) \end{aligned}$$

8. Conclusions

- The spiral of Theodorus (Th. of Cyrene, 465 - 398 B.C.) provides a wide field of challenges in theoretical and numerical mathematics:
- The monotonic solution of the corresponding functional equation was first given by Ph. Davis (1993), independently rediscovered by Heuvers, Moak and Boursaw (2000).
- The analytic continuation presented here seems to be new.
- A numerical challenge is the summation of slowly convergent series.
- As an efficient technique, summation by contour integration and numerical quadrature by the trapezoidal rule is suggested.
- The trapezoidal rule quickly integrates analytic functions over $\mathbb{R}$.
- The asymptotic expansion of the polar angle provides an alternate fast algorithm for evaluating the relevant mathematical functions.