

The Higher Derivatives Of The Inverse Tangent Function and Rapidly Convergent BBP-Type Formulas For π *

Kunle Adegoke[†], Olawanle Layeni[‡]

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Abstract

We give a closed formula for the n -th derivative of $\arctan x$. A new self consistent expansion for $\arctan x$ is also obtained and rapidly convergent series for π are derived.

1 Introduction

The derivation of the n -th derivative of $\arctan x$ is not straightforward (see e.g. [1, 2]). Also the computation of π and the problem of finding rapidly converging series for $\arctan x$ have remained interwoven. Numerous interesting series for π ranging from the Gregory-Leibniz [3] formula through the Machin-Like formulas [4] to the more recent BBP-Type formulas [5] are based directly or indirectly on rapidly convergent series for $\arctan x$. Of course there are also interesting series for π whose connections with $\arctan x$, if any, may not be obvious. Examples would be the numerous series for π , discovered by Ramanujan [6].

In the following sections we will give a closed formula for the n -th derivative of $\arctan x$. A new series expansion for $\arctan x$ will also be obtained and rapidly convergent series for π will be derived.

2 The n -th Derivative of $\arctan x$

We have the following result.

THEOREM 1. The function $f(x) = \arctan x$ possesses derivatives of all order for $x \in (-\infty, \infty)$. The n -th derivative is given by the formula

$$\frac{d^n}{dx^n} (\arctan x) = \frac{(-1)^{n-1}(n-1)!}{(1+x^2)^{n/2}} \sin \left(n \arcsin \left(\frac{1}{\sqrt{1+x^2}} \right) \right), \quad n = 1, 2, 3, \dots \quad (1)$$

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[†]Department of Physics, Obafemi Awolowo University, Ile-Ife, Nigeria

[‡]Department of Mathematics, Obafemi Awolowo University, Ile-Ife, Nigeria

PROOF. It is convenient to make the right hand side of the above equation more compact by writing

$$\sin \theta = \frac{1}{\sqrt{1+x^2}}.$$

The formula then becomes

$$\frac{d^n}{dx^n} (\arctan x) = (-1)^{n-1} (n-1)! \sin^n \theta \sin n\theta.$$

The existence of the derivatives follows from the analyticity of $\arctan x$ on the real line. The proof of formula (1) is by mathematical induction. Clearly, the theorem is true for $n = 1$. Suppose the theorem is true for $n = k$; that is, suppose

$$P_k : \frac{d^k}{dx^k} (\arctan x) = (-1)^{k-1} (k-1)! \sin^k \theta \sin k\theta. \quad (2)$$

We will show that the theorem is true for $n = k + 1$ whenever it is true for $n = k$. Differentiating both sides of (2) with respect to x and noting that $d\theta/dx = -\sin^2 \theta$ gives

$$\begin{aligned} \frac{d}{dx} \left[\frac{d^k}{dx^k} (\arctan x) \right] &= (-1)^k k! \sin^{k+1} \theta (\cos \theta \sin k\theta + \cos k\theta \sin \theta) \\ &= (-1)^k k! \sin^{k+1} \theta \sin(k+1)\theta. \end{aligned} \quad (3)$$

That is

$$P_{k+1} : \frac{d^{k+1}}{dx^{k+1}} (\arctan x) = (-1)^k k! \sin^{k+1} \theta \sin(k+1)\theta,$$

and the proof is complete.

3 A New Expansion for $\arctan x$

Perhaps the most well known series for $\arctan x$ is its Maclaurin's expansion

$$\begin{aligned} \arctan x &= \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+1}}{2n+1} \\ &= x - \frac{x^3}{3} + \frac{x^5}{5} - \frac{x^7}{7} + \dots \end{aligned} \quad (4)$$

Apart from its simplicity and elegance, series (4) as it stands has little computational value as its radius of convergence is small ($R = 1$) and the convergence is slow (logarithmic convergence) at the interesting endpoint $x = 1$. Note however that for $|x| < 1$, one finds roughly $n \log_{10}(x)$ decimals of $\arctan x$ after the n -th term, so that the convergence is linear. Euler transformation gives the form [7]:

$$\arctan x = \sum_{n=0}^{\infty} \frac{2^{2n} (n!)^2}{(2n+1)!} \frac{x^{2n+1}}{(1+x^2)^{n+1}}. \quad (5)$$

The ratio test establishes easily that the series (5) converges for all real x , giving $R = \infty$. Formula (5) exhibits linear convergence since

$$\lim_{n \rightarrow \infty} \frac{|u_{n+1} - \arctan x|}{|u_n - \arctan x|} = 1,$$

where

$$u_n = \frac{2^{2n}(n!)^2}{(2n+1)!} \frac{x^{2n+1}}{(1+x^2)^{n+1}}$$

is the n -th term of the series.

We now present a new self consistent series for $\arctan x$.

THEOREM 2. The function $f(x) = \arctan x$, $x \in (-\infty, \infty)$ has the self consistent expansion

$$\arctan x = \sum_{n=1}^{\infty} \frac{1}{n} \left(\frac{x^2}{1+x^2} \right)^{n/2} \sin \left(n \arcsin \frac{1}{\sqrt{1+x^2}} \right). \quad (6)$$

PROOF. Taylor's expansion for a function $f(x)$ which is analytic in an interval I which includes the point $x = 0$ may be written as

$$f(x) = f(0) - \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} x^n f^n(x). \quad (7)$$

Since $f(x) = \arctan x$ is analytic in $(-\infty, \infty)$, it has the series expansion given by (7). The derivatives are given by (1). The substitution of (1) in (7) gives (6) and the proof is complete.

The ratio test gives as condition for convergence of the series (6)

$$\left| \frac{x}{\sqrt{1+x^2}} \right| < 1,$$

a condition which is automatically fulfilled for all x in $(-\infty, \infty)$.

4 Rapidly Convergent Series for π

In the notation of section 2, Equation (6) can be written as

$$\frac{\pi}{2} - \theta = \sum_{n=1}^{\infty} \frac{1}{n} \cos^n \theta \sin n\theta. \quad (8)$$

A more general form of equation (8) can be found in [8]. Note that series (8) is linearly convergent, since the convergence rate μ is

$$\mu = \lim_{n \rightarrow \infty} \frac{|\cos^{n+1} \theta \sin(n+1)\theta / (n+1) - \pi/2 + \theta|}{|\cos^n \theta \sin(n\theta) / n - \pi/2 + \theta|} = 1.$$

What is remarkable about (8) is that careful choices of θ yield interesting series for π . For example, on setting $\theta = \pi/4$, we obtain the series

$$\frac{\pi}{4} = \sum_{n=1}^{\infty} \frac{1}{2^{n/2}n} \sin \frac{n\pi}{4}. \tag{9}$$

Contrary to appearance, the right hand side contains no surd and does not require the knowledge of π for evaluation, since $\sin(n\pi/4)$ can only take one of five possible values:

$$\sin \frac{n\pi}{4} = \begin{cases} -1 & n = 6, 14, 22, 30, \dots \\ -1/\sqrt{2} & n = 5, 7, 13, 15, \dots \\ 0 & n = 4, 8, 12, 16, \dots \\ 1/\sqrt{2} & n = 1, 3, 9, 11, \dots \\ 1 & n = 2, 10, 18, 26, \dots \end{cases}.$$

Thus (9) can be written as

$$\frac{\pi}{4} = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{4^n} \left[\frac{2}{4n-3} + \frac{1}{2n-1} + \frac{1}{4n-1} \right],$$

or better still, by switching the summation index

$$\pi = \sum_{n=0}^{\infty} \frac{(-1)^n}{4^n} \left[\frac{2}{4n+1} + \frac{2}{4n+2} + \frac{1}{4n+3} \right]. \tag{10}$$

Formula (10) is clearly a base 4 BBP [9]-Type formula. The original BBP formula

$$\pi = \sum_{n=0}^{\infty} \frac{1}{16^n} \left(\frac{4}{8n+1} - \frac{2}{8n+4} - \frac{1}{8n+5} - \frac{1}{8n+6} \right)$$

discovered using the PSLQ algorithm [10] allows the n -th hexadecimal digit of π to be computed without having to compute any of the previous digits and without requiring ultra high-precision [5]. Formula (10) has also been obtained earlier, using the same PSLQ algorithm and is listed as formula (14) in Bailey's compendium of known BBP-type formulas [11]. It must be stated that there is no apparent connection between our arctan expansion and the PSLQ algorithm.

An even more rapidly converging series (i.e. requiring fewer terms to achieve the same accuracy) for π can be derived by setting $\theta = \pi/3$ in (8), obtaining

$$\frac{\pi}{6} = \sum_{n=1}^{\infty} \frac{1}{2^n n} \sin \frac{n\pi}{3}.$$

Again since

$$\sin \frac{n\pi}{3} = \frac{\sqrt{3}}{2} \times \begin{cases} 1 & n = 1, 2, 7, 8, 13, 14, \dots \\ 0 & n = 0, 3, 6, 9, 12, 15, \dots \\ -1 & n = 4, 5, 10, 11, 16, 17, \dots \end{cases},$$

the above series can be written as

$$\frac{\pi}{6} = \frac{\sqrt{3}}{2} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{2^{3n}} \left[\frac{4}{3n-2} + \frac{2}{3n-1} \right].$$

That is

$$\pi = \frac{3\sqrt{3}}{8} \sum_{n=0}^{\infty} \frac{(-1)^n}{8^n} \left[\frac{4}{3n+1} + \frac{2}{3n+2} \right]. \quad (11)$$

For same accuracy, more terms are required of the Euler series ($x = 1$ in Equation (5))

$$\frac{\pi}{2} = 1 + \frac{1}{3} + \frac{1.2}{3.5} + \frac{1.2.3}{3.5.7} + \dots \quad (12)$$

than the series (11), a base 8 BBP-Type formula.

Although more terms of the series (10) are needed than of the series (11) and series (12) for the same accuracy, series (10) is computationally more convenient because the coefficients are rational. We can also obtain yet another converging series by setting $\theta = \pi/6$ in (8), obtaining

$$\frac{\pi}{3} = \sum_{n=1}^{\infty} \left(\frac{\sqrt{3}}{2} \right)^n \frac{1}{n} \sin \frac{n\pi}{6},$$

which when written out is

$$\begin{aligned} \pi = \left(\frac{3}{4} \right)^3 \sqrt{3} \sum_{n=0}^{\infty} (-1)^n \left(\frac{3}{4} \right)^{3n} & \left[\frac{16}{9} \frac{1}{(6n+1)} + \frac{8}{3} \frac{1}{(6n+2)} \right. \\ & \left. + \frac{8}{3} \frac{1}{(6n+3)} + \frac{2}{6n+4} + \frac{1}{6n+5} \right]. \end{aligned} \quad (13)$$

Series (13) (like (10), (11) and (12)) converges linearly to π . More terms of the series (13) are however required to achieve the same accuracy.

5 Conclusion

We have given a closed form formula for the n -th derivative of $\arctan x$:

$$\frac{d^n}{dx^n} (\arctan x) = \frac{(-1)^{n-1} (n-1)!}{(1+x^2)^{n/2}} \sin \left(n \arcsin \left(\frac{1}{\sqrt{1+x^2}} \right) \right), \quad n = 1, 2, 3, \dots$$

We also gave a new self consistent expansion for $\arctan x$, $x \in (-\infty, \infty)$:

$$\arctan x = \sum_{n=1}^{\infty} \frac{1}{n} \left(\frac{x^2}{1+x^2} \right)^{n/2} \sin \left(n \arcsin \frac{1}{\sqrt{1+x^2}} \right).$$

Finally we presented rapidly convergent BBP-Type series for π :

$$\pi = \sum_{n=0}^{\infty} \frac{(-1)^n}{4^n} \left[\frac{2}{4n+1} + \frac{2}{4n+2} + \frac{1}{4n+3} \right].$$

$$\pi = \frac{3\sqrt{3}}{8} \sum_{n=0}^{\infty} \frac{(-1)^n}{8^n} \left[\frac{4}{3n+1} + \frac{2}{3n+2} \right].$$

$$\pi = \left(\frac{3}{4}\right)^3 \sqrt{3} \sum_{n=0}^{\infty} (-1)^n \left(\frac{3}{4}\right)^{3n} \left[\frac{16}{9} \frac{1}{(6n+1)} + \frac{8}{3} \frac{1}{(6n+2)} \right. \\ \left. + \frac{8}{3} \frac{1}{(6n+3)} + \frac{2}{6n+4} + \frac{1}{6n+5} \right].$$

The generator of the BBP-Type series is the formula

$$\frac{\pi}{2} - \theta = \sum_{n=1}^{\infty} \frac{1}{n} \cos^n \theta \sin n\theta.$$

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