The higher derivatives of the inverse tangent function and rapidly convergent BBP-type formulas

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Abstract

We give a closed formula for the $n^{th}$ derivative of $\arctan x$. A new expansion for $\arctan x$ is also obtained and rapidly convergent series for $\pi$ and $\pi\sqrt{3}$ are derived.

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Keywords: $n^{th}$ derivative, arctan, BBP-type formulas, pi, mathematical induction, series expansion
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5 Summary

1 Introduction

The derivation of the $n^{th}$ derivative of $\arctan x$ is not straightforward (see e.g [1, 2]). Efficient numerical computation of $\pi$ and related constants is often dependent on finding rapidly converging series for the inverse tangent function. Numerous interesting series and identities for $\pi$, ranging from the Gregory-Leibniz [3] formula through the Machin-Like formulas [4] to the more recent BBP-type formulas [5], are derived by manipulating the inverse tangent function. Of course there are also interesting series for $\pi$ whose connections with the arctangent function may not be obvious. Examples would be the numerous series for $\pi$, discovered by Ramanujan [6].

In this paper 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 $\pi$ and $\pi\sqrt{3}$ 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 of $\arctan x$ is given by the formula

$$\frac{d^n}{dx^n} (\arctan x) = (-1)^{n-1}(n-1)! \sin \left[ n \arcsin \left( \frac{1}{\sqrt{1+x^2}} \right) \right], \quad n \in \mathbb{Z}^+.$$  

(2.1)

PROOF. It is convenient to make the right hand side of (2.1) more compact by writing

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

The formula then becomes

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

2
The existence of the derivatives follows from the analyticity of \( \arctan x \) on the real line. The proof of formula (2.1) is by mathematical induction. Clearly, the theorem is true for \( n = 1 \). Suppose the theorem is true for \( n = k \); that is, suppose

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

We will show that the theorem is true for \( n = k + 1 \) whenever it is true for \( n = k \).

Differentiating both sides of (2.2) with respect to \( x \) and noting that \( d\theta/dx = -\sin^2 \theta \), we have

\[
\frac{d}{dx} \left[ \frac{d^k}{dx^k} (\arctan x) \right] = (-1)^k k! \sin^{k+1} \theta (\cos \theta \sin k\theta + \cos k\theta \sin \theta) \\
= (-1)^k k! \sin^{k+1} \theta \sin(k+1)\theta ,
\]

so that

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

Thus \( P_k \Rightarrow P_{k+1} \) and the proof is complete.

3 A new expansion for \( \arctan x \)

Perhaps the most well known series for \( \arctan x \) is its Maclaurin expansion

\[
\arctan x = \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+1}}{2n + 1} = x - \frac{x^3}{3} + \frac{x^5}{5} - \frac{x^7}{7} + \cdots
\]

Apart from its simplicity and elegance, series (3.1) 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 \( x \), so that the convergence is linear. Euler transformation gives the form [7]:

\[
\arctan x = \sum_{n=0}^{\infty} \frac{2^{2n}(n!)^2}{(2n+1)!} \frac{x^{2n+1}}{(1 + x^2)^{n+1}}. \tag{3.2}
\]

The ratio test establishes easily that the series (3.2) converges for all real \( x \), giving \( R = \infty \). Formula (3.2) exhibits linear convergence.

We now present a new series for \( \arctan x \).

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

\[
\arctan x = \sum_{n=1}^{\infty} \frac{1}{n} \left( \frac{x^2}{1 + x^2} \right)^{n/2} \sin \left( n \arcsin \frac{1}{\sqrt{1 + x^2}} \right). \tag{3.3}
\]

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

\[
f(x) = f(0) - \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} x^n f^n(x). \tag{3.4}
\]

Since \( f(x) = \arctan x \) is analytic in \( (-\infty, \infty) \), it has the series expansion given by (3.4). The derivatives of \( \arctan x \) are given by (2.1). The substitution of (2.1) in (3.4) gives (3.3) and the proof is complete.

The ratio test gives as condition for convergence of the series (3.3)

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

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

4 Rapidly convergent series for \( \pi \) and \( \pi \sqrt{3} \)

In the notation of section 2, (3.3) can be written as

\[
\frac{\pi}{2} - \theta = \sum_{n=1}^{\infty} \frac{1}{n} \cos^n \theta \sin n\theta. \tag{4.1}
\]

A more general form of (4.1) can be found in [8]. What is remarkable about (4.1) is that careful choices of \( \theta \) yield interesting series for \( \pi \) and \( \pi \sqrt{3} \).
On setting $\theta = \pi/4$, we obtain the series

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

(4.2)

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

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

Thus (4.2) can be written as

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

or better still, by shifting the summation index

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

(4.3)

Formula (4.3) is a base 4 BBP \cite{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 \cite{10} allows the $n$th hexadecimal digit of $\pi$ to be computed without having to compute any of the previous digits and without requiring ultra high-precision \cite{5}. Formula (4.3) has also been obtained earlier and is listed as formula (16) in Bailey’s compendium of known BBP-type formulas \cite{11}.

A converging series for $\pi \sqrt{3}$ can be derived by setting $\theta = \pi/3$ in (4.1), obtaining

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

5
Again since
\[ \sin \frac{n\pi}{3} = \frac{\sqrt{3}}{2} \times \begin{cases} 
1, & n = 1, 2, 7, 8, 13, 14, \ldots \\
0, & n = 0, 3, 6, 9, 12, 15, \ldots \\
-1, & n = 4, 5, 10, 11, 16, 17, \ldots 
\end{cases}, \]
the above series can be written as
\[ \frac{\pi}{6} = \frac{\sqrt{3}}{2} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{2^{3n}} \left[ \frac{4}{3n-2} + \frac{2}{3n-1} \right], \]
so that we have
\[ \pi \sqrt{3} = \frac{9}{8} \sum_{n=0}^{\infty} \frac{(-1)^n}{8^n} \left[ \frac{4}{3n+1} + \frac{2}{3n+2} \right], \]
giving a base 8 BBP-type formula for \( \pi \sqrt{3} \).

We can obtain yet another converging series by setting \( \theta = \pi/6 \) in (4.1), 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
\[ \pi \sqrt{3} = \frac{9}{64} \sum_{n=0}^{\infty} (-1)^n \left( \frac{3}{4} \right)^n \left[ \frac{16}{(6n+1)} + \frac{24}{(6n+2)} + \frac{24}{(6n+3)} + \frac{18}{(6n+4)} + \frac{9}{(6n+5)} \right]. \]

We note that technically speaking (4.4) is not a BBP-type formula.

## 5 Summary

We have given a closed form formula for the \( n^{th} \) derivative of \( \arctan x \):
\[ \frac{d^n}{dx^n} (\arctan x) = \frac{(-1)^{n-1}(n-1)!}{(1+x^2)^{n/2}} \sin \left[ n \arcsin \left( \frac{1}{\sqrt{1+x^2}} \right) \right], \]
\( n = 1, 2, 3, \ldots \)
We also obtained a new 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 derived rapidly convergent series for \( \pi \) and \( \pi \sqrt{3} \):

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

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

and

\[
\pi \sqrt{3} = \frac{9}{64} \sum_{n=0}^{\infty} (-1)^n \left( \frac{3}{4} \right)^{3n} \left[ \frac{16}{(6n+1)} + \frac{24}{(6n+2)} \right.
\]

\[
+ \frac{24}{(6n+3)} + \frac{18}{6n+4} + \frac{9}{6n+5} \]

The generator of the BBP-type series is the formula

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

**Acknowledgments.**

KA is grateful to Prof. Angela Kunoth for encouragements. The authors wish to acknowledge the anonymous reviewer, whose useful comments helped to improve the quality of this work.

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