MAST90053 EXPERIMENTAL MATHEMATICS

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More on BBP formulas

This lecture, largely based on J. M. Borwein, Borwein, and Galway (2004), is devoted to some of the theory behind BBP formulas of the form

$$\alpha = P(s, b, n, A),$$

where

$$P(s, b, n, A) = \sum_{k \geq 0} \frac{1}{b^k} \sum_{j=1}^{n} \frac{a_j}{(nk + j)^s},$$

and $A = (a_1, \dots, a_n) \in \mathbb{Z}^n$. We will also write

$$P(s, b, n, A) = \sum_{j=1}^{n} a_j L(s, b, n, j)$$

and call $L(s, b, n, j)$ *BBP generators*.

If $s = 1$, we will call representations of the above form *logarithmic* because for $s = 1$ resembles the expansion of $-\log(1 - x)$:

$$-\log(1 - x) = \sum_{k \geq 1} \frac{x^k}{k}$$

By the same token, for general s it is called *polylogarithmic* due to the similarity of with the polylogarithm function $\mathrm{Li}_s(z)$ defined by

$$\mathrm{Li}_s(x) = \sum_{k \geq 1} \frac{x^k}{k^s}.$$

The two formulas we saw last week are of this form:

$$\log 2 = \sum_{k \geq 1} \frac{1}{k 2^k} = \frac{1}{2} P(1, 2, 1, (1)),$$

or, more generally,

$$\log\left(1 - \frac{1}{b^m}\right) = -\sum_{k \geq 1} \frac{1}{k b^{mk}} = -b^{-m} P(1, b^m, 1, (1)),$$

and

$$\begin{aligned} \pi &= \sum_{k=0}^{\infty} \frac{1}{16^k} \left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6} \right) \\ &= P(1, 16, 8, (4, 0, 0, -2, -1, -1, 0, 0)) \end{aligned}$$

The existence of a BBP formula to the base 2 for $\log 2$ already implies the existence of a base 2 formula for many other logarithms. For instance, a formula for $\log 3$ can be obtained by the following reasoning:

$$\begin{aligned}
\log 3 = 2\log 2 + \log\left(1 - \frac{1}{4}\right) &= 2\sum_{k\geq 1}\frac{1}{k2^k} - \sum_{k\geq 1}\frac{1}{k4^k} \\
&= \frac{1}{2}\sum_{k\geq 0}\frac{1}{4^k}\left(\frac{2}{2k+1} + \frac{1}{2k+2}\right) - \frac{1}{4}\sum_{k\geq 0}\frac{1}{4^k}\left(\frac{2}{2k+2}\right) \\
&= \sum_{k\geq 0}\frac{1}{4^k}\left(\frac{1}{2k+1}\right) \\
&= P(1,4,2,(1,0))
\end{aligned}$$

Where we made use of the fact that, given $m \in \mathbb{N}$, a BBP formula to the base b can be rewritten as a BBP formula to the base b^m by taking terms m at a time:

$$\sum_{k\geq 0}\frac{p(k)}{q(k)}b^{-k} = \sum_{k\geq 0}\left(\sum_{j=0}^{m-1}\frac{p(mk+j)}{b^j q(mk+j)}\right)b^{-mk}$$

By combining the formulas for $\log(1-2^{-m})$, we can obtain a BBP formula to the base 2 for $\log q$ for any integer q that can be written as

$$q = \frac{(2^{a_1}-1)(2^{a_2}-1)\cdots(2^{a_h}-1)}{(2^{b_1}-1)(2^{b_2}-1)\cdots(2^{b_j}-1)}.$$

Machin-type BBP formulas

The original Machin's formula (1706) is the following identity:

$$\pi/4 = 4\arctan(1/5) - \arctan(1/239).$$

Machin used this formula to compute 100 digits of π. A *Machin-type formula* for π is a formula expressing π as a $\mathbb{Z}$-linear combination of arctangents. In 2002, Yasumasa Kanada announced the record computation of 1.24 trillion decimal digits of π, using the identities

$$\begin{aligned}
\pi &= 48\arctan(1/49) + 128\arctan(1/57) \\
&\qquad - 20\arctan(1/239) + 48\arctan(1/110443) \\
\pi &= 176\arctan(1/57) + 28\arctan(1/239) \\
&\qquad - 48\arctan(1/682) + 96\arctan(1/12943)
\end{aligned}$$

One way to understand these indentities is to observe that

$$\arctan(y/x) = \operatorname{Im}\log(x+iy).$$

Machin's formula is therefore a consequence of the factorisation $(2 + 2i) = (5 + i)^4(230 + i)$. Similarly, Kanada's identities can be verified by observing that the products

$$(49 + i)^{48}(57 + i)^{128}(239 + i)^{-20}(110443 + i)^{48}$$

and

$$(57 + i)^{176}(239 + i)^{28}(682 + i)^{-48}(12943 + i)^{96}$$

both yield negative rational numbers.

Machin-type BBP generators

Combining the log expansion with the above observation we define the *Machin-type BBP generators* to be BBP generators of the form

$$\begin{aligned}\arctan(-b^{-m}) = \operatorname{Im}\log(1 - b^{-m}) &= -b^{-m}\sum_{k\geq 0}\frac{(-1)^k}{2k+1}b^{-2mk} \\ &= b^{-3m}P(1, b^{4m}, 4, (-b^{2m}, 0, 1, 0)).\end{aligned}$$

where we assume that $b \geq 2$ and not a proper power. Setting $x = \pm 2^{-m}$ in the series expansion for $\arctan(x/(1+x))$ yields a binary BBP formula which is distinct from the generators above. Thus, when $b = 2$ we use additional generators (called *Aurifeuillian*) of the form

$$\arctan\left(\frac{1}{1 \pm 2^m}\right) = \operatorname{Im}\log(1 \pm (1 + i)2^{-m}).$$

EXERCISE 1. Express the above generators in terms of Bailey's generators $P(s, b, n, A)$.

Note that the three generators $\arctan(-b^{-m})$ and $\arctan(1/(1 \pm 2^m)$ are not independent because

$$\operatorname{Im}\log\left(1 + (1 + i)2^{-m}\right) = \operatorname{Im}\log\left(1 - i2^{1-2m}\right) - \operatorname{Im}\log\left(1 - (1 + i)2^{-m}\right).$$

Finding Machin-type BBP arctangent formulas

Using the formulas from the previous section, a BBP formula for $\pi/4$ follows almost immediately:

$$\pi/4 = -\arctan(-1) = 2^{-4}P(1, 2^4, 8, [8, 8, 4, 0, -2, -2, -1, 0]),$$

which is the case $r = -1/4$ of the formula

$$\begin{aligned}\pi = \sum_{k=0}^{\infty}\frac{1}{16^k}\Bigg(&\frac{4+8r}{8k+1} - \frac{8r}{8k+2} - \frac{4r}{8k+3} - \frac{2+8r}{8k+4} \\ &- \frac{1+2r}{8k+5} - \frac{1+2r}{8k+6} + \frac{r}{8k+7}\Bigg),\end{aligned}$$

seen last week.

Other binary Machin-type BBP formulas for $\pi/4$ can be found by looking for products of the form

$$z = \prod_j (2^{a_j} - i)^{n_j} \prod_j (2^{b_j} - 1 - i)^{m_j} = \alpha(1+i)$$

for some $\alpha \in \mathbb{Q}$. The first factor corresponds to the Machin-type generators with $b = 2$ and the second factor to the Aurifeuillian generators.

A hand search for additional formulas soon reveals that

$$\begin{aligned}(2-i)(3-i) &= 5 - 5i\\ (2-i)^2(7+i) &= 25 - 25i\\ (3-i)^2(7-i) &= 50 - 50i\end{aligned}$$

corresponding to the formulas

$$\begin{aligned}\pi/4 &= \arctan(1/2) + \arctan(1/3)\\ \pi/4 &= 2\arctan(1/2) - \arctan(1/7)\\ \pi/4 &= 2\arctan(1/2) + \arctan(1/7)\end{aligned}$$

Carl Størmer proved in 1897 that these, together with Machin's formula, are the only four non-trivial integral solutions to

$$m \arctan(1/u) + n \arctan(1/v) = k\pi/4$$

Similarly, one can look for binary Machin-type BBP formulas for arctangents with arguments different from $1/(1 \pm 2^m)$

Exercise 2. Prove that $\arctan(1/6) = \arctan(1/5) - \arctan(1/31)$.

Non-binary Machin-type arctangent formula for π

Here we investigate the possibility of a non-binary formula of for π of Machin-type (there are no Aurifeuillian generators for $b > 2$). We first need some preliminary definitions.

Definition 1. Given fixed $b > 1$, we say that a prime p is a *primitive prime factor* of $b^m - 1$ if p divides $b^m - 1$ but does not divide any $b^n - 1$ for $n < m$. In other words, m is the least integer such that p divides $b^m - 1$.

Theorem 1. Bang (1886). The only cases where $b^m - 1$ has no primitive prime factors are when $b = 2$, $m = 6$, (therefore $b^m - 1 = 3^2 7$); and when $b = 2^N - 1$, $N \in \mathbb{N}$, $m = 2$, (therefore $b^m - 1 = 2^{N+1}(2^{N-1} - 1)$).

Bang's Theorem can be used as an exclusion criterium for binary arctangent Machin-type formulas for π:

THEOREM 2. Given $b > 2$ and not a proper power, there is no $\mathbb{Q}$-linear b-ary Machin-type BBP arctangent formula for π.

If π were to have a $\mathbb{Q}$-linear Machin-type BBP arctangent formula, it would be of the form

$$n\pi = \sum_{m=1}^{M} n_m \operatorname{Im}\log(b^m - i),$$

where $n \in \mathbb{N}$, $n_m \in \mathbb{Z}$, and $M \geq 1$, $n_M \neq 0$. This implies that

$$\prod_{m=1}^{M} (b^m - i)^{n_m} = \alpha e^{ni\pi} \in \mathbb{Q}$$

for some $\alpha \in \mathbb{Q}$, $\alpha \neq 0$. For any $b > 2$ and not a proper power, it follows from Bang's Theorem that $b^{4M} - 1$ has a primitive prime factor, say p. Furthermore, p must be odd since $p = 2$ can only be a primitive prime factor of $b^m - 1$ when b is odd and $m = 1$. Since p is a primitive prime factor of it does not divide $b^{2M} - 1$, and hence must divide $b^{2M} + 1 = (b^M - i)(b^M + i)$. Now p cannot divide both $(b^M - i)$ and $(b^M + i)$ since this would give the contradiction that p divides $(b^M - i) - (b^M + i) = 2i$. It follows that p factors as $p = \mathfrak{p}\bar{\mathfrak{p}}$ over $\mathbb{Z}[i]$, where $\mathfrak{p}$ and $\bar{\mathfrak{p}}$ are conjugate primes in $\mathbb{Z}[i]$, and with exactly one of $\mathfrak{p}$, $\bar{\mathfrak{p}}$ dividing $b^M - i$. Furthermore, for $m < M$ neither $\mathfrak{p}$ nor $\bar{\mathfrak{p}}$ can divide $b^m - i$ since this would imply that p divides $b^{4m} - 1$ with $m < M$, contradicting the fact that p is a primitive prime factor of $b^{4M} - 1$. So, we conclude that the left hand side of is divisible by exactly one of $\mathfrak{p}$, $\bar{\mathfrak{p}}$ but not by the other, while any non-zero number in $\mathbb{Q}$ if divisible by either $\mathfrak{p}$ or $\bar{\mathfrak{p}}$ is also divisible by the other. Hence we arrive at a contradiction.

References

Borwein, Jonathan M, David Borwein, and William F Galway. 2004. "Finding and Excluding B-Ary Machin-Type Individual Digit Formulae." *Canadian Journal of Mathematics* 56 (5). THE UNIVERSITY OF TORONTO PRESS INC.: 897–925.