Integral approximations to π with nonnegative integrands

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One of the more beautiful results related to approximating π is the integral

$$I = \int_0^1 \frac{x^4 (1-x)^4}{1+x^2} \, dx = \frac{22}{7} - \pi. \tag{1}$$

Since the integrand is nonnegative on the interval [0, 1], this shows that π is strictly less than 22/7, the well known approximation to π . Here we shall look at some features of this integral, including error bounds and a related series expansion. Then, we present a number of generalizations, including a new series approximation to π where each term adds as many digits of accuracy as you wish. We conclude by presenting a number of related integral results for other continued fraction convergents of π .

1 The classic integral

Proving (1) is not difficult, if perhaps somewhat tedious. A partial fraction decomposition leads to

$$\frac{x^4(1-x)^4}{1+x^2} = x^6 - 4x^5 + 5x^4 - 4x^2 + 4 - \frac{4}{1+x^2},$$
(2)

and integration immediately gives us that

$$\int_0^1 \frac{x^4(1-x)^4}{1+x^2} \, dx = \frac{1}{7} - \frac{2}{3} + 1 - \frac{4}{3} + 4 - 4\frac{\pi}{4}$$

from which (1) immediately follows. An alternative is to use the substitution $x = \tan \theta$, leading to

$$\int_{0}^{1} \frac{x^{4}(1-x)^{4}}{1+x^{2}} dx = \int_{0}^{\pi/4} \frac{\tan^{4} \theta (1-\tan \theta)^{4}}{\sec^{2} \theta} \sec^{2} \theta d\theta$$
$$= \int_{0}^{\pi/4} \tan^{4} \theta - 4 \tan^{5} \theta + 6 \tan^{6} \theta - 4 \tan^{7} \theta + \tan^{8} \theta d\theta.$$

This can be solved using the recurrence relation $(\tan^n \theta = \tan^{n-2} \theta(\sec^2 \theta - 1))$

$$\int_0^{\pi/4} \tan^n \theta \, d\theta = \frac{1}{n-1} - \int_0^{\pi/4} \tan^{n-2} \theta \, d\theta,$$

with

$$\int_0^{\pi/4} d\theta = \frac{\pi}{4}, \quad \int_0^{\pi/4} \tan \theta \, d\theta = \ln \sqrt{2},$$

which returns the required result after some algebra. Of course, the simplest approach today is to simply verify (1) using a symbolic manipulation package.

The earliest statement of this result that we are aware of is Dalzell [5] in 1944. Proving (1) was a question in a University of Sydney examination in November 1960 (Borwein *et al.* [3]), and it was apparently shown by Kurt Mahler to his students in the mid 1960's. Proving (1) was also the first question in the William Lowell Putnam mathematical competition of October 1968, as published by McKay [8] in 1969. In 1971, Dalzell [6] again derived (1) in a larger work published in the Cambridge student journal *Eureka*. This paper is the one most often cited in context with the result (1) (e.g. Backhouse [1] and Borwein *et al.* [3]). It was also presented without reference in Cornwell [4] in 1980. A more recent reference is Medina [9].

1.1 Error estimation

As well as showing $22/7 > \pi$, we can use this integral result (1) to get bounds on the error. One approach, following Nield [10] (The actual paper misspells the name as Neild, which is reproduced by MathSciNet) is to note that since $x(1-x) \le 1/4$ and $1 + x^2 \ge 1$ on [0, 1] with equality only at the endpoints, the integrand takes maximum value $(1/4)^2 = 1/256$. Combined with the fact that $22/7 - \pi$ is positive, we get the error bound

$$\frac{5625}{1792} = \frac{22}{7} - \frac{1}{256} < \pi < \frac{22}{7}.$$

However, a better bound can be found by noting that $1 < 1 + x^2 < 2$ for $x \in (0,1)$, and $\int_0^1 x^4 (1-x)^4 dx = 1/630$ (as in Dalzell [5, 6] and Nield [11]). Then

$$\frac{1}{1260} < \frac{22}{7} - \pi < \frac{1}{630} \quad \text{or} \quad \frac{22}{7} - \frac{1}{630} < \pi < \frac{22}{7} - \frac{1}{1260}$$

The interval [1979/630,3959/1260] is of width 7.94 $\times 10^{-4},$ and is not centered at $\pi.$

1.2 Series expansion

Dalzell [5] also provides a series expansion for π based upon (2), which is included in Borwein *et al.* [3] as an example. After gathering the two pieces with $1 + x^2$ as the denominator, we can write

$$\frac{1}{1+x^2} = \frac{x^6 - 4x^5 + 5x^4 - 4x^2 + 4}{4+x^4(1-x)^4} \quad \text{or} \quad \frac{4}{1+x^2} = \frac{x^6 - 4x^5 + 5x^4 - 4x^2 + 4}{1+x^4(1-x)^4/4}.$$

Integrating both sides between 0 and 1 and using the Taylor series expansion for 1/(1+t) leads to

$$\pi = \sum_{k=0}^{\infty} \left(-\frac{1}{4}\right)^k \int_0^1 (x^6 - 4x^5 + 5x^4 - 4x^2 + 4)x^{4k}(1-x)^{4k} \, dx.$$
(3)

Applying integration by parts n times reducing the coefficient of (1 - x), we have

$$\int_0^1 x^m (1-x)^n \, dx = \frac{m! n!}{(m+n+1)!},\tag{4}$$

where m and n are nonnegative integers, which when applied to (3) gives

$$\pi = \sum_{k=0}^{\infty} \left(-\frac{1}{4} \right)^{k} \left[\frac{(4k)!(4k+6)!}{(8k+7)!} - \frac{4(4k)!(4k+5)!}{(8k+6)!} + \frac{5(4k)!(4k+4)!}{(8k+5)!} - \frac{4(4k)!(4k+2)!}{(8k+3)!} + \frac{4(4k)!^{2}}{(8k+1)!} \right].$$
(5)

The sequence (5) is equivalent to that derived in Dalzell [5, 6] and Borwein *et al.* [3], but written in a different form. There the sixth order polynomial in (3) is recognized to be unchanged when x is replaced by 1 - x, and so additional algebra is performed to reformulate the integral in (3) as

$$\int_{0}^{1} \left(3 + x(1-x) - \frac{1}{2}x^{2}(1-x)^{2} - x^{3}(1-x)^{3}\right) x^{4k}(1-x)^{4k} dx = \frac{3(4k)!^{2}}{(8k+1)!} + \frac{(4k+1)!^{2}}{(8k+3)!} - \frac{(4k+2)!^{2}}{2(8k+5)!} - \frac{(4k+3)!^{2}}{(8k+7)!}, \tag{6}$$

where we have applied (4) with m = n several times. To show that (5) and (6) are equivalent, it is easiest to factor both of them, and incidentally get a cleaner solution. In both cases, start by giving them the common denominator (8k+7)!, and take the common factor $(4k)!^2$. It quickly becomes apparent that (4k + 1)(4k + 2)(4k + 3) is also a common factor, and we find that both expressions lead to

$$\pi = \sum_{k=0}^{\infty} (-1)^k 4^{2-k} \frac{(4k)!(4k+3)!}{(8k+7)!} (820k^3 + 1533k^2 + 902k + 165)$$

$$= \frac{22}{7} - \frac{19}{15015} + \frac{543}{594914320} - \frac{77}{104187267600} + \cdots.$$
(7)

The convergence rate can be found by applying Stirling's approximation for the factorials and taking the ratios of successive terms, giving that each term has magnitude roughly 1/1024 of the previous term, or roughly 3 decimal digits of accuracy are added per term. Using just the first two terms, and knowing that the error when truncating an alternating series with terms decreasing in magnitude is less than or equal to the absolute value of the first term in the truncated part, we can form the bound

$$\frac{22}{7} - \frac{19}{15015} \le \pi \le \frac{22}{7} + \frac{19}{15015},\tag{8}$$

which is of width 2.53×10^{-3} . This result is poorer than bound from the previous section, but if we use three terms, then

$$\frac{22}{7} - \frac{19}{15015} - \frac{543}{594914320} \le \pi \le \frac{22}{7} - \frac{19}{15015} + \frac{543}{594914320},\tag{9}$$

which is a bound of width 1.83×10^{-6} , an improvement.

We can make one more perhaps artificial use of the series (7). By taking the first k terms to the left hand side, we can show $\pi \in [a, b]$ as in (8) and (9). If z is then some number near π , we can rewrite the bound as $\pi \in [z - (z - a), z - (z - b)]$. Applying this to (8) and (9) with z = 355/113, the next good rational approximation of π , we get

$$\pi \in \left[\frac{355}{113} - \frac{118}{10^8}, \frac{355}{113} + \frac{253}{10^5}\right] \quad \text{and} \quad \pi \in \left[\frac{355}{113} - \frac{210}{10^8}, \frac{355}{113} - \frac{266}{10^9}\right].$$

2 Related families of integrals

There turn out to be a number of families of integrals that are similar in style to (1). The most obvious is originally due to Nield [10] in 1982, who introduces

$$I_{4n} = \int_0^1 \frac{x^{4n} (1-x)^{4n}}{1+x^2} \, dx \tag{10}$$

for positive integers n. Then I from (1) is equivalent to I_4 . Medina [9] has investigated this set of integrals in detail, where the upper bound in the integral has been replaced by x, and polynomial approximations to $\arctan(x)$ with rational coefficients are developed. From our perspective, one of the most useful results he gives is the closed form expression

$$\frac{x^{4n}(1-x)^{4n}}{1+x^2} = (x^6 - 4x^5 + 5x^4 - 4x^2 + 4)\sum_{k=0}^{n-1} (-4)^{n-1-k} x^{4k} (1-x)^{4k} + \frac{(-4)^n}{1+x^2}.$$
(11)

While not proven explicitly in [9], this can easily be proven by mathematical induction. Integrating (11) using (4) and simplifying leads to

$$\frac{(-1)^n}{4^{n-1}} \int_0^1 \frac{x^{4n}(1-x)^{4n}}{1+x^2} dx = \pi - \sum_{k=0}^{n-1} (-1)^k \frac{2^{4-2k}(4k)!(4k+3)!}{(8k+7)!} \times (820k^3 + 1533k^2 + 902k + 165),$$

where the integral and simplification was already done earlier for Dalzell's series expansion. So in fact the closed form expression for $(-1)^n I_{4n}/4^{n-1}$ is equivalent to the error when approximating π by a truncated version of Dalzell's series expansion! Every increase in n will increase by roughly two and a half the number of digits of accuracy in the approximation to π . It is less accurate due to the $1/4^{n-1}$ term.

In 1995, Backhouse [1] generalized (1) to

$$I_{m,n} = \int_0^1 \frac{x^m (1-x)^n}{1+x^2} \, dx = a + b\pi + c \ln(2), \tag{12}$$

where a, b and c are rationals that depend on the positive integers m and n, and a and b have opposite sign. In this case, $I \equiv I_{4,4}$. Backhouse [1] showed that if $2m - n \equiv 0 \pmod{4}$, then c = 0 and approximations to π result. In what follows we shall assume that this is the case. An integral equal to $a + b\pi$ gives the approximation -a/b for π . As m and n increase, the integrand becomes increasingly flat (Backhouse calls them "pancake functions") and the approximations to π improve, as well. Unfortunately, there is no straightforward formula relating a and b directly to m and n as in the I_{4n} case. However, Weisstein [13] at least states the result

$$I_{m,n} = 2^{-(m+n+1)} \sqrt{\pi} \Gamma(m+1) \Gamma(n+1) \times {}_{3}F_{2}\left(1, \frac{m+1}{2}, \frac{m+2}{2}; \frac{m+n+2}{2}; \frac{m+n+3}{2}; -1\right).$$

2.1 Error estimation

We previously saw that error bounds for I could be found using the bounds $1 \le 1 + x^2 \le 2$. The same approach for $I_{m,n}$ directly leads to

$$\frac{m!n!}{2(m+n+1)!} < a+b\pi = \int_0^1 \frac{x^m(1-x)^n}{1+x^2} \, dx < \frac{m!n!}{(m+n+1)!},$$

where a and b are the rationals depending on m and n. As m and n increase, the bounds on the error decrease with reasonable rapidity.

2.2 Series expansion

Given the closed form expression (11), we can follow the same process as Dalzell to produce series expansions for π , with a specific value of n leading to

$$\pi = \sum_{m=0}^{\infty} \sum_{k=0}^{n-1} (-4)^{-nm-k} \int_0^1 (x^6 - 4x^5 + 5x^4 - 4x^2 + 4) x^{4(k+nm)} (1-x)^{4(k+nm)} dx,$$
(13)

which generalizes (3). Evaluating the integrals as before leads to

$$\pi = \sum_{m=0}^{\infty} \sum_{k=0}^{n-1} (-1)^{\alpha} 4^{2-\alpha} \frac{(4\alpha)!(4\alpha+3)!}{(8\alpha+7)!} (820\alpha^3 + 1533\alpha^2 + 902\alpha + 165), \quad (14)$$

where $\alpha = k + nm$. With n = 1, (14) is exactly Dalzell's expansion (7). With n = 2 we have

$$\pi = \sum_{m=0}^{\infty} 4^{2-2m} \left[\frac{(8m)!(8m+3)!}{(16m+7)!} (6560m^3 + 6132m^2 + 1804m + 165) - \frac{(8m+4)!(8m+7)!}{(16m+15)!} (1640m^3 + 3993m^2 + 3214m + 855) \right]$$
$$= \frac{47171}{15015} + \frac{16553}{18150270600} + \frac{64615651}{102659859353904652800} + \cdots$$

Note that this is not an alternating series, and each term is roughly $1/2^{20}$ of the previous, or roughly 6 digits of accuracy are added per term.

There is no reason why we can't take n as large as we like. While this increases the amount of work to find each term in the series, each term is roughly $1/2^{10n}$ the size of the previous term, or roughly 3n digits of accuracy are added with each term. In principle, there is no reason why a series where each term adds one hundred digits or more of accuracy cannot be explicitly written down from (14) with $n \geq 33$.

3 Integrals leading to convergents

The main reason for appreciating the elegance of (1) surely is due to its approximating π by 22/7, the classic and most well-known rational approximation both within and outside the mathematics community. The number 22/7 is particularly good because it is better than other rational approximation p/q for q < 57. In fact it is one of the *convergents* of the continued fraction approximation to π , the first few of which are 3, 22/7, 333/106, 355/113, 103993/33102 and 104348/33215. There are many excellent texts on continued fractions, including Olds [12]. A natural question, then, is whether there are integrals similar to the ones shown here that lead to other convergents of π .

Unfortunately, none of the integrals considered so far lead to approximations to π related to the other convergents of π . The 22/7 in (1) must be considered a happy coincidence. However, Lucas [7] developed a set of integrals with nonnegative integrands that equalled $355/113 - \pi$, where 355/113is the next particularly good approximation to π . Here, we generalize those results, and show how integrals with nonnegative integrands can be formed for $z - \pi$ (if $z > \pi$) or $\pi - z$ (if $z < \pi$), with any real z.

We begin by noting that $I_{m,n}$ from (12) is a combination of multiples of 1, π , and ln 2. Now consider the related integral

$$I'_{m,n} = \int_0^1 \frac{x^m (1-x)^n (a+bx+cx^2)}{1+x^2} \, dx,$$

which can be evaluated as a combination of 1, π and ln 2, where the coefficients depend on a, b and c. If we want the integral to equal $z - \pi$, this leads to a set of three linear equations in the three unknowns. A solution leads to an integral of the appropriate form. However, it does not guarantee that the integrand is nonnegative. To do so, we need to increase m and n until we get a solution where $a + bx + cx^2 \ge 0$ for $x \in [0, 1]$. The closer z is to π , the larger m and n will need to be. As m and n increase, the coefficients a, b and c become increasingly large, and so a "best" solution can be found, in the sense that the number of characters required to form the integrand is minimal. Lucas [7] only considered integrals leading to $355/113 - \pi$ using the symbolic toolbox within Matlab to evaluate the integrals. A more effective approach is to use Maple, and the code in figure 1 can be used for $355/113 - \pi$. Changing 355/113 to other values is straightforward. Using code like this we can easily show (1) is the simplest approximation using 22/7. Experimentation suggests that the simplest results for other continued fractions are

$$\int_{0}^{1} \frac{x^{5}(1-x)^{6}(197+462x^{2})}{530(1+x^{2})} dx = \pi - \frac{333}{106},$$
$$\int_{0}^{1} \frac{x^{8}(1-x)^{8}(25+816x^{2})}{3164(1+x^{2})} dx = \frac{355}{113} - \pi,$$
$$\int_{0}^{1} \frac{x^{14}(1-x)^{12}(124360+77159x^{2})}{755216(1+x^{2})} dx = \pi - \frac{103993}{33102},$$

and

$$\int_0^1 \frac{x^{12}(1-x)^{12}(1349-1060x^2)}{38544(1+x^2)} \, dx = \frac{104348}{33215} - \pi$$

```
for m from 1 to 12 do
  for n from 1 to 12 do
    x:='x': a:='a': b:='b': c:='c':
    sol:=int(x^m*(1-x)^n*(a+b*x+c*x^2)/(1+x^2),x=0..1):
    out:=op(sol): eq1:=0: eq2:=0: eq3:=0:
    for i from 1 to nops(sol) do
      if type(out[i],Or(name,rational&*name,name&*rational)) then
        eq1:=eq1+out[i]:
      elif type(out[i]/Pi,Or(name,rational&*name,name&*rational)) then
        eq2:=eq2+out[i]/Pi:
      else
        eq3:=eq3+out[i]/log(2):
      end if;
    end do:
    assign(solve({eq1=355/113,eq2=-1,eq3=0})):
    assume(x>=0,x<=1); print(m,n,a,b,c,is(a+b*x+c*x^2>=0));
  end do:
end do:
```

Figure 1: Maple code to find coefficients of integrals that approximate π

We conclude with the somewhat sillier results

$$\int_0^1 \frac{x^8 (1-x)^6 (61+250x+61x^2)}{500(1+x^2)} \, dx = 3.14160 - \pi,\tag{15}$$

and

$$\int_0^1 \frac{x^9 (1-x)^6 (944+6569x^2)}{11250(1+x^2)} \, dx = \pi - 3.14159,\tag{16}$$

that can be combined to prove that $3.14159 < \pi < 3.14160$.

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References

- N. Backhouse, Note 79.36, Pancake functions and approximations to π, Math. Gazette 79 (1995), 371–374.
- [2] F. Beukers, A rational approach to π , Nieuw Arch. Wiskd. (5) 1(4) (2000), 372–379.
- [3] J.M. Borwein, D.H. Bailey and R. Girgensohn *Experimentation in Mathematics: Computational Paths to Discovery*, A.K. Peters, Ltd., 2004.
- [4] R. Cornwell, A proof that Pi is not 22/7, New Zealand Math. Mag. 17 (1980), 127.
- [5] D.P. Dalzell, On 22/7, J. London Math. Soc. 19 (1944), 133–134.
- [6] D.P. Dalzell, On 22/7 and 355/113, Eureka: the Archimedian's Journal 34 (1971), 10–13.
- [7] S.K. Lucas, Integral proofs that $355/113 > \pi$, Gazzette Aust. Math. Soc. **32** (2005), 263–266.
- [8] J.H. McKay, The William Lowell Putnam mathematical competition, Amer. Math. Monthly, **76**(8) (1969), 909–915.
- [9] H.A. Medina, A sequence of polynomials for approximating inverse tangent, Amer. Math. Monthly, 113(2) (2006), 156–161.
- [10] D.A. Nield (misspelled Neild in the article), Rational approximations to Pi, New Zealand Math. Mag. 18 (1982), 99–100.
- [11] D.A. Nield, Rational approximations to Pi: a further comment, New Zealand Math. Mag. 19 (1982), 60–61.
- [12] C.D. Olds, *Continued Fractions*, Random House, 1963.
- [13] E.W. Weisstein, Pi formulas, from MathWorld-A Wolfram Web Resource, http://mathworld.wolfram.com/PiFormulas.html, May 2007.