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Rational Approximations to π

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Abstract. Using an IBM 1130 computer, we have generated the first 20,000 partial quotients in the ordinary continued-fraction representation of π.

1. Introduction. With the aid of high speed computers, it has become possible to determine to very high accuracy the decimal representation of particularly interesting irrational numbers. Shanks and Wrench [1] have found the first 100,000D of π, and this information can be used to generate a large section of its ordinary continued fraction representation. Using an IBM 1130 computer, we have obtained the first 20,000 partial quotients of π. The computation sheds some light on the problems of generating a huge section of the continued fraction of an irrational number. It is advantageous to generate a continued fraction, section by section, rather than to generate the partial quotients (p.q.'s) singly. Moreover, the size of the sections should be chosen carefully.

To illustrate the method used, we present an example: Euler's constant, $\gamma =$ 0.5772156649, to 10 decimal places. We work with a pair of numbers A and B; A is set initially to zero, $B = 0.5772156649$, and the sum $A + B$ is formed. The fractional part of $A + B$ is stored in B or A, respectively, according as there is or is not a carry into the integer portion. The process continues with the current A and B:

0.0000000000	A	
0.5772156649	B	
0.5772156649	A	$\cdots\cdots\ a_1 = 1$
0.1544313298	B	$\cdots\cdots\ a_2 = 1$
0.7316469947	A	$\cdots\cdots\ a_3 = 2$
0.8860783245	A	
0.0405096543	B	$\cdots\cdots\ a_4 = 1$
0.9265879788	A	$\cdots\cdots\ a_5 = 2$
0.9670976331	A	
0.0076072874	B	$\cdots\cdots\ a_6 = 1$
0.9747049205	A	$\cdots\cdots\ a_7 = 4$
0.9823122079	A	
0.9899194953	A	
0.9975267827	A	
0.0051340701	B	

The number of consecutive A's and B's in the list is recorded, and we obtain 1, 1, 2, 1, 2, 1, 4, $\cdots$, which is the start of the continued fraction representation of γ. Of

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course, the integers a_i ($i \geqq 1$) relate to $\bar{\gamma} = 0.5772156649$ rather than to γ, but the first 12 a_i's are the same for both numbers. An exceptional case arises, however, when $B = 0$ is obtained, i.e. the continued fraction terminates. Depending on whether zero comes at the end of a sequence of B's or A's, it should be labelled as B or A, respectively. Thus, in the latter case, 1.0 is regarded as the infinite decimal $0.99 \cdots$.

The above process has two obvious defects. First, in the event of a large a_i, many additions have to be performed to obtain it. Secondly, to obtain a large number of p.q.'s, each A and B must have a correspondingly large number of digits. When these numbers become too large to keep in the working store of the computer, the efficiency falls off sharply.

2. Mathematical Background. There is a close connection between continued fractions and the concept of best rational approximation [2]. The convergents $p_i/q_i = [a_1, a_2, \cdots, a_{i-1}]^{**}$ ($i \geqq 2$) to a real number θ ($0 < \theta \leqq 1$) are also best rational approximations (BRA's) to θ, in the sense that $|q_i\theta - p_i| < |q\theta - p|$ for all non-negative integers $q < q_i$ and all p. We can define $(p_0, q_0) = (1, 0)$ and $(p_1, q_1) = (0, 1)$ to start the sequence of pairs (p_i, q_i), and a_i may be generated from the recurrence relation:

$$(q_{i+1}\theta - p_{i+1}) = a_i(q_i\theta - p_i) + (q_{i-1}\theta - p_{i-1}) \qquad (i \geqq 1), \tag{2.1}$$

in which the terms $(q_i\theta - p_i)$ alternate in sign. Denoting $q_i\theta - p_i$ by $\phi_i(\theta)$, $\phi_i(\theta)$ is added repeatedly to $\phi_{i-1}(\theta)$. The last number in the sequence $\phi_i + \phi_{i-1}$, $2\phi_i + \phi_{i-1}$, $3\phi_i + \phi_{i-1}, \cdots$, with the same sign as $\phi_{i-1}(\theta)$, is $\phi_{i+1}(\theta)$. a_i is obtained in the process.

The algorithm in Section 1 differs in one detail from that above. $\phi_{2k}(\theta)$ is replaced by $\psi_{2k}(\theta) \equiv 1 + \phi_{2k}(\theta)$, and $\psi_{2k+1}(\theta) = \phi_{2k+1}(\theta)$ ($k \geqq 0$). This dispenses with negative numbers. The algorithm (2.1) becomes:

$$\psi_{i+1}(\theta) = \{a_i\psi_i(\theta) + \psi_{i-1}(\theta)\}, \qquad (i \geqq 1), \tag{2.2}$$

where $\{\ \}$ denotes fractional part. The sequence (ψ_{2k}) increases monotonically and ultimately consists of numbers of the form $0.999 \cdots$, while the sequence (ψ_{2k+1}) decreases monotonically to zero.

Finally, in attempting to generate the continued fraction of an irrational number, we will need a result such as the following:

THEOREM I. *If p_{2k-1}/q_{2k-1} and p_{2k}/q_{2k} ($k \geqq 1$) are successive BRA's to $\bar{\theta}$ ($0 < \bar{\theta} < 1$), and if there exist positive integers m and m' ($m \geqq m'$) such that*

(i) $10^{-2m} > \theta - \bar{\theta} > 0$ and

(ii) $|q_{2k}\bar{\theta} - p_{2k}| > 10^{-m'}$,

then p_{2k-1}/q_{2k-1} and p_{2k}/q_{2k} are BRA's to θ. Also $q_{2k} < 10^m$.

Proof. The proof depends on two well-known results:

(1) If p_{2k-1}/q_{2k-1} and p_{2k}/q_{2k} are BRA's to $\bar{\theta}$, then they are BRA's for all x such that $(p_{2k-1} + p_{2k})/(q_{2k-1} + q_{2k}) \leqq x \leqq p_{2k}/q_{2k}$.

$$\frac{1}{a_{2k}q_{2k}} > |q_{2k}\bar{\theta} - p_{2k}| = (p_{2k} - q_{2k}\bar{\theta}) > \frac{1}{(a_{2k}+1)q_{2k}}. \tag{2}$$

Thus, $1/q_{2k} > p_{2k} - q_{2k}\bar{\theta} > 10^{-m'}$, i.e. $10^{m'} > q_{2k}$. Multiplying inequalities yields

** Denotes a terminating continued fraction.

$p_{2k}/q_{2k} - \bar{\theta} > 10^{-2m'}$. By (i) $p_{2k}/q_{2k} - \bar{\theta} > \theta - \bar{\theta}$, which implies that $p_{2k}/q_{2k} > \theta > \bar{\theta} \geqq (p_{2k-1} + p_{2k})/(q_{2k-1} + q_{2k})$.

COROLLARY. *Under the hypotheses of Theorem* I, *the p.q.'s* $a_1, a_2, \cdots, a_{2k-1}$ *are common to both* $\bar{\theta}$ *and* θ. *Stated simply, the result is*: *Take the first* 2*m digits of* $\psi_0(\theta)$ *and* $\psi_1(\theta)$, *then the* a_i*'s* $(i \geqq 1)$, *generated from the truncated numbers, are correct for* θ, *until a type-A number is obtained with m nines immediately after the decimal point.*

In the next section, this result is modified to a form which is used repeatedly in the program.

3. Improved Method. The algorithm of Section 1 is unsuitable for generating a large number of p.q.'s for the reasons given there. However, its main defects are easily removed.

Instead of adding ψ_i to ψ_{i-1}, one can add $10^{\alpha}\psi_i$, where $\alpha \geqq 0$ is the smallest integer such that $\{10^{\alpha+1}\psi_i + \psi_{i-1}\}$ and ψ_i are of the same type (A or B). The process continues with $\psi'_{i-1} = \{10^{\alpha}\psi_i + \psi_{i-1}\}$ instead of ψ_{i-1} until ψ_{i+1} is obtained. If t is the time required to find ψ_{i+1} by the original method, then the time by the modified method is approximately $\log_{10} t$. The process is further speeded up by using, instead of the algorithm (2.2), the following result [3]:

$$\phi_i(\theta) = p_i\phi_0(\theta) + q_i\phi_1(\theta) \qquad (i \geqq 2), \tag{3.1}$$

or its equivalent:

$$\psi_i(\theta) = \{p_i\psi_0(\theta) + q_i\psi_1(\theta)\}. \tag{3.2}$$

An approximation $\bar{\theta}$ to θ is used to generate $a_1, a_2, \cdots, a_{i-1}$; p_{i-1}, q_{i-1}; p_i and q_i for some i (odd integer). Equation (3.2) then yields $\psi_{i-1}(\theta)$ and $\psi_i(\theta)$ to full accuracy. Next, a new pair ψ_0 and ψ_1 is obtained from ψ_{i-1} and ψ_i, by multiplying the latter pair by the least power of 10 sufficient to remove all nines immediately following the decimal point of ψ_{i-1}, and then taking fractional parts. The partial quotients $a_i, a_{i+1}, \cdots$ for θ are just the p.q.'s for the new number $\psi_1/(1 - \psi_0)$ and are obtained by using truncated versions of ψ_0 and ψ_1. So the process is repeated with each new $\theta = \psi_1/(1 - \psi_0)$. However, suppose $\bar{\psi}_0$ and $\bar{\psi}_1$ denote, respectively, ψ_0 and ψ_1 truncated to $2m$ digits, then all that is known about the difference $\theta - \bar{\theta}$ is that $10^{-2m+2} > \theta - \bar{\theta} \geqq 0$. The test for whether θ and $\bar{\theta}$ have the same p.q.'s is provided, not by Theorem I, but by the following:

THEOREM II. *If* $\bar{\psi}_0$ *and* $\bar{\psi}_1$ *are given by the first* 2*m decimal digits of* ψ_0 *and* ψ_1, *respectively, if the sequences* $(\bar{\psi}_{i+1})$ *and* (a_i) $(i \geqq 1)$ *are generated in the usual way, and if* $1 - \bar{\psi}_{2k} > 10^{-m'}$ $(m' \leqq m - 1)$, *then* $a_1, a_2, \cdots, a_{2k-1}$ *are p.q.'s of* $\theta = \psi_1/(1 - \psi_0)$.

It should be noted that a $\bar{\psi}_2$ may be obtained which is so close to one that no progress can be made. For large m, however, this possibility becomes so unlikely as to be negligible.

4. Program. We have generated the first 21,230 p.q.'s of π using a program based on the analysis of Sections 2 and 3, and using the first 25,000 decimal places of π obtained from the table of Wrench and Shanks [1]. In fact, the program used binary numbers and was written in IBM 1130 machine language in which a word will hold integers $<2^{16}$.

We can estimate the theoretical time for the main program. Let c_i $(1 \leqq i \leqq 5)$

denote certain constants for the program by which N p.q.'s are generated in sections of M p.q.'s, the numbers A and B in the main store (disc) being revised after each section. We start with a $2n$ digit number θ and use approximations to it (and to each new θ) with $2m$ digits. $N/M \simeq n/m$. Three basic operations are each repeated n/m times:

(i) Each p.q. takes an average computation time $a + bm$. Each section of M p.q.'s is generated in time $c_1 m + c_2 m^2$.

(ii) The four multipliers in the algorithm (3.2) are computed in an average time $c_3 m^2$.

(iii) To update the disc once requires an average time $n(c_4 m^2 + c_5 m)/m$, where $c_4 mn$ is the time for multiplications, and $c_5 n$ the time for transfers between the disc and working area (core).

Total time $T = n[c_1 + (c_2 + c_3)m + c_4 n + c_5 n/m]$. For fixed n, T is least when $m^2 = c_5 n/(c_2 + c_3)$. In our program, $m = 640$ binary digits ($n \simeq 40{,}000$) was chosen to use up available core space and, due to the expected size of c_5, is still likely to be less than the optimum value. In any event, the main program generated just over 20,000 p.q.'s in 4.6 hours. The binary conversion of data and conversion of our results into decimal took a further one hour.

As a check against machine errors, the program was run twice and as an additional safeguard, different values of m' (Theorem II) were used on each occasion. A printout of the input data has been checked repeatedly against the original table [1].

5. Results. Because of its length, a table of the first 21,230 p.q.'s of π is not published here, but has been placed in the UMT file of this journal, together with the first 3470 p.q.'s of γ obtained while testing the program. (See Review **23**, p. 403, this issue.) The frequency with which the integer n ($n \leqq 10$) appears as a partial quotient in these tables is compared in Table 1 with $(\log [(n + 1)^2/n(n + 2)])/(\log 2)$, the cor-

TABLE 1

n	*Frequency of occurrence of n*: 21,230 p.q.'s of π	3470 p.q.'s of γ	*Theoretical frequency distribution,* $\left(\log \dfrac{(n+1)^2}{n(n+2)}\right) \Big/ (\log 2)$
1	.4188	.4225	.4150
2	.1694	.1696	.1699
3	.0890	.0905	.0931
4	.0577	.0550	.0589
5	.0437	.0435	.0406
6	.0278	.0320	.0297
7	.0236	.0210	.0227
8	.0189	.0202	.0179
9	.0140	.0118	.0144
10	.0120	.0124	.0119

TABLE 2

The partial quotients > 2000 in the first 21,230 p.q.'s of π

i	a_i
431	20,776
15,543	19,055
20,276	18,127
3,811	8,277
8,719	7,444
19,223	4,767
20,358	4,415
12,426	4,264
3,777	2,159
6,209	2,050

responding frequency distribution for 'almost every' irrational number (see, for example, [4]). We have also listed those p.q.'s so far obtained for π which exceed 2000. See Table 2. The largest, $a_{431} = 20{,}776$, occurs comparatively early.

After 20,831 p.q.'s were generated, the disc underwent one of its periodic revisions. We found that $2^{-35,579} > B > 2^{-35,580}$, $2^{-35,580} > 1 - A > 2^{-35,581}$, and $a_{20,831} = 1$. From these numbers we obtain bounds for $q_{20,831}$: $2^{35,578} < q_{20,831} < 2^{35,580}$. We also find that 21,422 decimal places of π are sufficient to generate $a_{20,830}$, but 21,419 decimal places are not enough. The first statement depends on the following:

PROPOSITION. *If p_{2k+1}/q_{2k+1} is a BRA to θ, and if $2^{-2m} > \theta - \bar{\theta} > 0$ and $|q_{2k+1}\theta - p_{2k+1}| > 2^{-m}$, then p_{2k+1}/q_{2k+1} is a BRA to $\bar{\theta}$.*

The proof is similar to that of Theorem I.

Here θ is a truncated version of π. The convergent $(p/q)_{20,831}$ for θ, and approximately the next 400 convergents, hold for π. Then $(p/q)_{20,831}$ also holds for $\bar{\theta} = \pi$ truncated to 71,160 binary places (or 21,422 decimal places). However, $\bar{\theta} = \pi$ truncated to 21,419 decimal places does not lie between

$$\left(\frac{p}{q}\right)_{20,831} \quad \text{and} \quad \frac{p_{20,830} + p_{20,831}}{q_{20,830} + q_{20,831}}.$$

It was shown by Levy (see [4, p. 75]) that, for almost every real number,

$$\operatorname*{Lim}_{k \to \infty} \frac{1}{k} \log q_k = \frac{\pi^2}{12 \log 2} = 1.1865 \cdots .$$

For π and $k = 20{,}831$, we have $(1/k) \log q_k = 1.1838 \cdots$.

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