An Iterative Method for Approximating Square Roots

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Introduction Mathematicians have been approximating the square roots of non-square integers with rational numbers for thousands of years. Many ingenious schemes have been used to generate these approximations and a good deal of interesting number theory has been discovered in the process. After reviewing some of these historical attempts and some of the number theory involved, we present an iterative procedure for approximating square roots which is based on an observation of M. A. Grant [3].

Some early approximations The Babylonians may have used the approximation formula

$$(a^2+h)^{1/2} \approx a + \frac{h}{2a}, \qquad 0 < h < a^2 \quad [2, \text{p. } 33].$$

The fact that this is a reasonable approximation is easily seen when we use the first two terms the binomial series

$$(1+x)^{1/2} = 1 + \sum_{n=1}^{\infty} \frac{1/2(1/2-1)\cdots(1/2-n+1)}{n!}x^n, \qquad |x| < 1,$$

with $x = h/a^2$, which gives us

$$\left(1+\frac{h}{a^2}\right)^{1/2} \approx 1 + \frac{1}{2}\frac{h}{a^2}.$$

Multiplying both sides of this equation by a gives us the Babylonian approximation. Taking $a=4$ and $h=1$, we see that $33/8$ is a Babylonian approximation of $\sqrt{17}$.

Heron of Alexandria (perhaps A.D. 50–100, [2, p. 157]) took an approximation a to $\sqrt{d}$ and then improved it by computing

$$\frac{a+\dfrac{d}{a}}{2}.$$

Notice that both a and d/a are approximations to $\sqrt{d}$. Since one of a or d/a is larger than $\sqrt{d}$ while the other is smaller than $\sqrt{d}$, the average of the two will be a better estimate. For example, with $a=4$, the next approximation, to $\sqrt{17}$ is $33/8$. This method is easily iterated and is used in some computers even today.

The Renaissance algebraist Rafael Bombelli is generally credited as the first to study continued fractions and the first mathematician to employ continued fractions to approximate $\sqrt{d}$.

We say that a rational number p/q is a "good approximation" of an irrational number ξ if

$$\left|\xi - \frac{p}{q}\right| < \frac{1}{q^2}.$$

For irrational numbers there are infinitely many such pairs of rational numbers. The set of all such good rational approximations for a given irrational number ξ is intimately related to the continued fraction expansion of ξ. In the next section we will develop the interplay between the "good" approximations of ξ and the continued fraction expansion of ξ.

More recently, M. A. Grant [3] demonstrated a method of approximating $\sqrt{d}$ by evaluating a sequence of rational functions at a certain rational point. His method is computationally simple and leads to very good approximations of $\sqrt{d}$. These approximations, in some cases, are good enough that one wonders if there is a connection between Grant's approximations and continued fractions. Happily, it turns out that an interesting connection exists between Grant's approximations and the theory of continued fractions. By exploiting this connection, we find an algorithm for producing approximations that is iterative and produces exceedingly good approximations to $\sqrt{d}$.

Continued fractions By a finite continued fraction, we mean a fraction of the form

$$a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \ddots + \cfrac{1}{a_{n-1} + \cfrac{1}{a_n}}}}.$$

Since this notation is cumbersome, this expression is denoted by $[a_0; a_1, \ldots, a_n]$. If all of the numbers $a_0, \ldots, a_n$ are integers, the continued fraction is called simple. Clearly a finite simple continued fraction is always rational. By the infinite simple continued fraction $[a_0; a_1, a_2, \ldots]$ we mean the limit of the sequence of rational numbers $a_0, [a_0; a_1], [a_0; a_1, a_2], \ldots$. That is,

$$[a_0; a_1, \ldots] = \lim_{n \to \infty} [a_0; a_1, \ldots, a_n].$$

The fraction $[a_0; a_1, \ldots, a_j]$ is called the jth convergent to $[a_0; a_1, \ldots]$ and is denoted by c_j. When we write $[a_0; a_1, \ldots, \overline{a_{k+1}, \ldots, a_{k+n}}]$, the line over $a_{k+1}, \ldots, a_{k+n}$ indicates that this block of integers is repeated over and over. Such an infinite continued fraction is called periodic, and we say that the period of the continued fraction has length n. To illustrate all of this notation, let us look at $[1; \overline{1, 2}]$, which represents the number

$$\alpha = 1 + \cfrac{1}{1 + \cfrac{1}{2 + \cfrac{1}{1 + \cfrac{1}{2}_{\ddots}}}} \tag{1}$$

What is the value of α? If we look carefully at (1), we see that

$$\alpha = 1 + \cfrac{1}{1 + \cfrac{1}{1 + \left(1 + \cfrac{1}{2 + \cdots}\right)}}$$

$$= 1 + \cfrac{1}{1 + \cfrac{1}{1 + \alpha}}.$$

After a little bit of algebra, one obtains $\alpha^2 = 3$ and since α is positive, $\alpha = \sqrt{3}$. Thus $\sqrt{3}$ is represented by the periodic continued fraction $[1; \overline{1,2}]$. The second convergent to $\sqrt{3}$ is

$$c_2 = [1;1,2] = 1 + \frac{1}{1 + 1/2} = \frac{5}{3}$$

while the third convergent is

$$c_3 = [1;1,2,1] = \frac{7}{4}.$$

As it turns out, all infinite simple continued fractions are irrational numbers. Also, every periodic simple continued fraction is an irrational root of a quadratic equation and conversely, every such irrational root has an infinite periodic simple continued fraction expansion.

In fact it is easy to find the continued fraction expansion of any irrational number. Let [ ] represent the greatest integer function. Then if x_0 is irrational, successively compute

$$x_1 = \frac{1}{x_0 - [x_0]}$$
$$\vdots$$
$$x_{j+1} = \frac{1}{x_j - [x_j]}, \quad \text{and}$$

take $a_n = [x_n]$. Then $x_0 = [a_0; a_1, \dots]$.

For example using this algorithm, we can compute the first three convergents to $\sqrt{17}$. We have $a_0 = 4$, $a_1 = 8$ and $a_2 = 8$ and so the first three convergents to $\sqrt{17}$ are

$$\frac{4}{1}, \frac{33}{8}, \quad \text{and} \quad \frac{268}{65}.$$

Two classical theorems [e.g. 4, theorems 171 and 184] relate irrational numbers to the convergents of continued fractions. One theorem tells us that if ξ is an irrational number, then the convergents to ξ are good approximations to ξ ($|\xi - p/q| < 1/q^2$). While the other theorem says that if p/q is a sufficiently good approximation to ξ ($|\xi - p/q| < 1/2q^2$) then p/q is a convergent to ξ.

Pells equation The connection between Grant's approximations and continued fractions involves "Pell's equation." Given a positive integer d, Pell's equation is satisfied by finding integers x and y such that

$$x^2 - dy^2 = 1. \tag{2}$$

If we take $x = \pm 1$ and $y = 0$ we get a trivial solution of this equation regardless of the value of d. If d is the square of an integer, say $d = n^2$, then

$$1 = x^2 - dy^2 = (x + ny)(x - ny),$$

which means that both $x + ny$ and $x - ny$ have to be ± 1 and since

$$x = \frac{(x + ny) + (x - ny)}{2},$$

we see that $x = \pm 1$ so $y = 0$ and so this is again the trivial solution of (2). Thus the only interesting cases of Pell's equation are when d is a nonsquare integer. Henceforth we restrict our attention to the case when d is a nonsquare integer.

Fermat was the first to state that for such d, the Pell equation has an infinite number of solutions but he did not provide a proof. This assertion was probably quite surprising to mathematicians of the time since there are cases with small d when the smallest solutions (x, y) are quite large. For example when $d = 13$, the smallest solution (x, y) is the pair (649, 180) while for $d = 29$ the smallest solution is $(x, y) = (9801, 1820)$.

We will require the following lemmas which relate the study of continued fractions and Pell's equation. These lemmas may be found in any of several standard number theory texts [e.g., **1**]. Remember that in each of these lemmas, d is a nonsquare positive integer.

LEMMA 1. *If (p, q) is a positive solution to $p^2 - dq^2 = 1$, then p/q is a convergent of the continued fraction expansion of $\sqrt{d}$.*

LEMMA 2. *Let p_k/q_k be the convergents of the continued fraction expansions of $\sqrt{d}$, and let n be the period of the continued fraction expansion for $\sqrt{d}$.*

1) *If n is even, then all positive solutions of $x^2 - dy^2 = 1$ are given by $x = p_{kn-1}$ and $y = q_{kn-1}$ $(k = 1, 2, 3, \ldots)$.*

2) *If n is odd, then all positive solutions of $x^2 - dy^2 = 1$ are given by $x = p_{2kn-1}$ and $y = q_{2kn-1}$ $(k = 1, 2, 3, \ldots)$.*

LEMMA 3. *If (x_1, y_1) is the smallest positive solution of $x^2 - dy^2 = 1$, then every positive solution of the equation is given by (x_j, y_j), where x_j and y_j are the integers defined by $x_j + y_j\sqrt{d} = (x_1 + y_1\sqrt{d})^j$.*

Before considering examples illustrating these ideas, we observe that the last two lemmas provide different descriptions of the solutions to Pell's equation. Since the solution sequences are both increasing and exhaustive, these two descriptions are, in fact, the same. Consequently, using the notation of Lemmas 2 and 3, we have

COROLLARY 1. *If n is even, then $x_k = p_{nk-1}$ and $y_k = q_{nk-1}$. If n is odd, then $x_k = p_{2nk-1}$ and $y_k = q_{2nk-1}$.*

Let us illustrate all of this with a pair of examples. Using the continued fraction algorithm described earlier, one can quickly find that $\sqrt{7} = [2; \overline{1, 1, 1, 4}]$ and $\sqrt{17} = [4; \overline{8}]$. Lemma 1 tells us that since $8^2 - 7 \cdot 3^2 = 1$, $8/3$ is a convergent to $\sqrt{7}$ and indeed $8/3 = [2; 1, 1, 1] = c_3$. Since the period in the partial fraction expansion of $\sqrt{7}$ is 4, Lemma 2 (part one) tells us that the convergents of $\sqrt{7}$ whose numerators and denominators give solution to Pells equation are $c_3, c_7, c_{11}, \ldots$. Similarly Lemma 2 (part 2) says that the convergents of $\sqrt{17}$ which give rise to solutions of Pell's equation are $c_1, c_3, c_5, \ldots$ since the period of $[4; \overline{8}]$ is one. Finally, Lemma 3 tells us that all of the convergents of $\sqrt{7}$ which give solutions to Pell's equation are defined by collecting terms in

$$x_j + y_j\sqrt{d} = (8 + 3\sqrt{7})^j.$$

And so the second smallest solution to the Pellian equation $x^2 - 7y^2 = 1$, which we already know to be c_7 by Lemma 2, is found by collecting terms of $(8 + 3\sqrt{7})^2$, thus

$$x_2 + y_2\sqrt{7} = (127 + 48\sqrt{7}),$$

i.e. $x_2 = 127$ and $y_2 = 48$ so we know that $c_7 = 127/48$. A quick calculation verifies this. Similarly, the convergent c_3 to $\sqrt{17}$ can be found by collecting the terms of $(33 + 8\sqrt{17})^2$ since $c_1 = 33/8$ gives the smallest positive solution of Pell's equation.

Approximation to $\sqrt{d}$ Grant makes a first approximation $x = p/q$ to $\sqrt{d}$ under the restriction $[\sqrt{d}] < x < [\sqrt{d}] + 1$, where [ ] again denotes the greatest integer function. With this choice of x, $0 < (x - \sqrt{d}) < 1$, and so $(x - \sqrt{d})^n \to 0$ as $n \to \infty$. If we expand $(x - \sqrt{d})^n \approx 0$ using the binomial theorem, we can solve for $\sqrt{d}$. For example,

$$(x - \sqrt{d})^4 \approx 0 \quad \text{so}$$

$$\sqrt{d} \approx \frac{x^4 + 6dx^2 + d^2}{4x^3 + 4dx}. \tag{3}$$

After choosing an approximation to $\sqrt{d}$, Grant improves his approximation by evaluating expressions like (3) for successively higher powers of $(x - \sqrt{d})$.

The examples of approximations that Grant provides are sometimes convergents to $\sqrt{d}$ and sometimes not. As we shall see, if we start with a convergent that gives a positive solution to Pell's equation, we may iterate this procedure and obtain a convergent to $\sqrt{d}$ after each iteration.

Grant uses only even powers $(x - \sqrt{d})^{2n}$ for his expansions. Although this is not necessary, it simplifies his exposition, and for the same reason we also adopt this simplification. Expanding $(x - \sqrt{d})^{2j} \approx 0$ and solving for $\sqrt{d}$, we obtain,

$$\sqrt{d} \approx \frac{\sum_{i=0}^{j} \binom{2j}{2i} x^{2i} d^{j-i}}{\sum_{i=0}^{j-1} \binom{2j}{2i+1} x^{2i+1} d^{j-i-1}}. \tag{4}$$

Let us denote the rational function obtained by manipulating $(x - \sqrt{d})^k$ in the above manner by $f_k(x)$. The right-hand side of the example in (3) above is thus denoted by $f_4(x)$ and Grant's method of improving the first approximation x to $\sqrt{d}$ involves successively computing the values of $f_2(x)$, $f_4(x)$, etc.

As it happens, the values $f_2(x)$, $f_4(x)$, etc. are not necessarily convergents of $\sqrt{d}$ and each successive approximation requires the computation of a new polynomial. At this point, we take a different tack. We fix a value of k, take a convergent x that gives a positive solution to Pell's equation, and then successively evaluate $f_k(x)$, $f_k(f_k(x))$, etc. Given this choice of x, the successive values are always convergents to $\sqrt{d}$.

The following theorem makes this statement precise.

THEOREM 1. *Let d be a nonsquare positive integer, k an even integer, and p/q a convergent to $\sqrt{d}$ such that (p, q) is a solution (x, y) of $x^2 - dy^2 = \pm 1$. Denote $f_k(p/q)$ by P/Q, then P/Q is also a convergent to $\sqrt{d}$ with (P, Q) a solution of Pell's equation.*

Proof. It is straightforward to show that

$$P^2 - dQ^2 = (p^2 - dq^2)^k \tag{5}$$

if we see the identity

$$\sum_{i=1}^{2j}\binom{2v}{i}\binom{2v}{2j-i}(-1)^i=(-1)^j\binom{2v}{j}.$$

We can see that the identity is true by comparing the coefficients of x^{2j} in $(1-x^2)^{2v}$ and $(1-x)^{2v}(1+x)^{2v}$. Returning to (5), we see that the value of P^2-dQ^2 must be 1 since $p^2-dq^2=\pm 1$ and k is even. Thus (P,Q) satisfies Pell's equation and so by Lemma 1, P/Q is a convergent to $\sqrt{d}$.

Notice that if k were odd, we would not be able to start with solutions (p,q) to $x^2-dy^2=-1$. In any case, since (P,Q) is a solution to Pell's equation, the process may be iterated with each step producing convergents to $\sqrt{d}$.

The next natural question to ask is, of course, "if p/q is the jth convergent of $\sqrt{d}$, then which convergent is $f_k(p/q)=P/Q$?" The answer is,

THEOREM 2. *Let d be a nonsquare positive integer and suppose that p/q is the jth convergent to $\sqrt{d}$ and that (p,q) is a positive solution to Pell's equation. Then $f_k(p/q)$ is the $[k(j+1)-1]$st convergent to $\sqrt{d}$.*

Proof. Again denote $f_k(p/q)$ by P/Q and the period of the continued fraction expansion by n. If p/q is the jth convergent to $\sqrt{d}$ and (p,q) is a positive solution of Pell's equation, then $j=mn-1$ for some m (if n is even) or $j=2mn-1$ for some m (if n is odd) by Lemma 2. In either case, by Lemma 3

$$p+q\sqrt{d}=\left(x_1+y_1\sqrt{d}\right)^m \tag{6}$$

since (p,q) is the mth positive solution of Pell's equation. By the previous theorem P/Q is also a convergent to $\sqrt{d}$ and a positive solution of Pell's equation. Say $P/Q=c_r$, then as before $r=an-1$ for some a (if n is even) or $r=2an-1$ for some a (if n is odd). In either case,

$$P+Q\sqrt{d}=\left(x_1+y_1\sqrt{d}\right)^a. \tag{7}$$

Now notice in equation (4) that $k=2j$ and if we let $x=p/q$ and multiply numerator and denominator by q^k, the resulting quotient is P/Q. Thus an alternative way to define P and Q would be to use the equation

$$P+Q\sqrt{d}=\left(p+q\sqrt{d}\right)^k.$$

Plugging equation (6) into this expression and equating with (7), we see that $a=mk$. Thus, for even n

$$\begin{aligned} r &= mkn-1\\ &= k(mn-1)+k-1\\ &= kj+k-1\\ &= k(j+1)-1. \end{aligned}$$

A similar calculation for odd n produces the same result and so P/Q is the $k[(j+1)-1]$st convergent to $\sqrt{d}$.

To illustrate this, we begin with Heron's approximation of $33/8$ for $\sqrt{17}$. As we have seen, $\sqrt{17}=[4;\bar{8}]$. Since $33/8$ is the first convergent to $\sqrt{17}$, Theorem 2 tells us that $f_4(33/8)$ is c_7, the seventh convergent to $\sqrt{17}$. With the aid of the computer, we have

$$f_4(c_1) = c_7 = \frac{9478657}{2298192}.$$

Iterating once produces

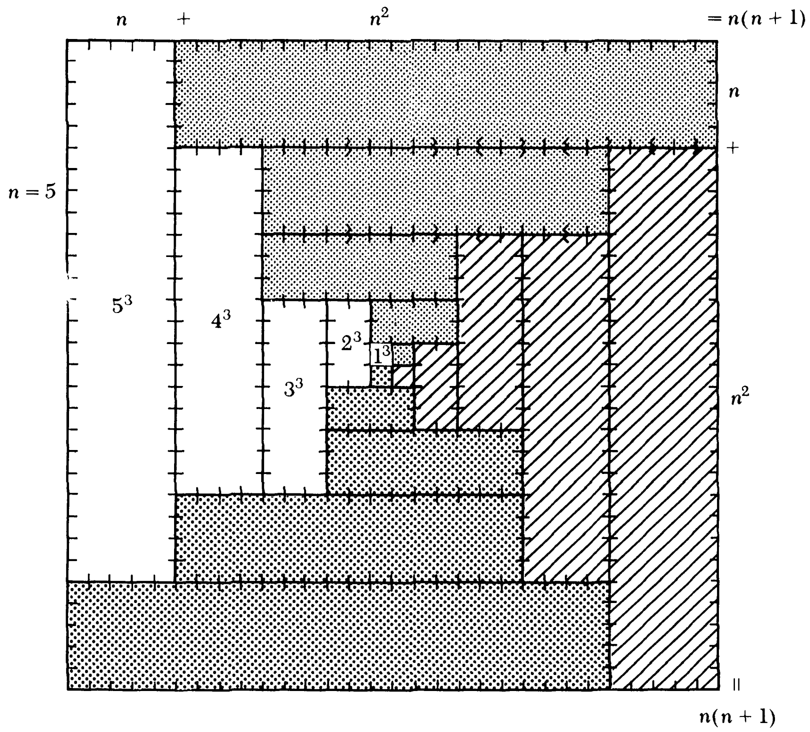
$$f_4(c_7) = c_{31} = \frac{64576903826545426454350012417}{15662199732482357532660158592}.$$

REFERENCES

1. D. M. Burton, *Elementary Number Theory*, Allyn and Bacon, 1980.
2. H. Eves, *An Introduction to the History of Mathematics*, Holt, Rinehart and Winston, 1969.
3. M. A. Grant, Approximation square roots, Note 66.36, *Math. Gaz.* (October 1982), 230–231.
4. G. H. Hardy and E. M. Wright, *An Introduction to the Theory of Numbers*, Oxford, 1960.

Proof without Words:

$$1^3 + 2^3 + 3^3 + 4^3 + \cdots + n^3 = \frac{\{n(n+1)\}^2}{4}$$



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