BEST APPROXIMATIONS OF $\sqrt{D}$

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ABSTRACT. For $D > 0$, not a square, we show that there are best approximations of the first kind to $\sqrt{D}$ that are not convergents to the simple continued fraction expansion of $\sqrt{D}$. We also show that if a/b is a best approximation of the first kind to $\sqrt{D}$ then $|a^2 - Db^2| \leq D$.

1. Introduction

Our main goal is to prove that there are best approximations of the first kind to $\sqrt{D}$ that are not convergents to the simple continued fraction expansion of $\sqrt{D}$. Specifically, we will show that if $\{t, u\}$ is any solution to $x^2 - Dy^2 = 1$, then for $0 \leq j < \sqrt{D} - 1$

$$\frac{Du + jt}{t + ju} \tag{1}$$

is a best approximation of the first kind to $\sqrt{D}$ and is not a convergent to the continued fraction expansion of $\sqrt{D}$. Similarly, if $D \geq 5$ and $\{t, u\}$ is any solution to $x^2 - Dy^2 = -1$, then for $1 \leq j < \sqrt{D}$, (1) is a best approximation of the first kind to $\sqrt{D}$ and is not a convergent to the continued fraction expansion of $\sqrt{D}$.

We also show that if a/b is a best approximation of the first kind to $\sqrt{D}$ then $|a^2 - Db^2| \leq D$.

2. PQa algorithm

We make great use of simple continued fractions below. The PQa algorithm computes the (simple) continued fraction expansion of the quadratic irrational $(P_0 + \sqrt{D})/Q_0$ for certain P_0, Q_0, D, and it computes some auxiliary variables.

Date: March 22, 2009.

Let P_0, Q_0, D be integers so that $Q_0 \neq 0$, $D > 0$ is not a square, and $P_0^2 \equiv D \pmod{Q_0}$. We are mainly interested in $\sqrt{D}$, so for all of our applications below, $P_0 = 0$ and $Q_0 = 1$. Set

$$A_{-2} = 0,\ A_{-1} = 1,$$
$$B_{-2} = 1,\ B_{-1} = 0,$$
$$G_{-2} = -P_0, \text{ and } G_{-1} = Q_0.$$

For $i \geq 0$ set

$$a_i = \left\lfloor (P_i + \sqrt{D})/Q_i \right\rfloor,$$
$$A_i = a_i A_{i-1} + A_{i-2},$$
$$B_i = a_i B_{i-1} + B_{i-2},$$
$$G_i = a_i G_{i-1} + G_{i-2},$$

and for $i \geq 1$ set

$$P_i = a_{i-1} Q_{i-1} - P_{i-1} \text{ and}$$
$$Q_i = (D - P_i^2)/Q_{i-1}.$$

Each of these variables will be an integer for all indices for which they are defined. A key output of this algorithm is the sequence a_0, a_1, a_2, ... which gives the continued fraction expansion of $\xi_0 = (P_0 + \sqrt{D})/Q_0$. That is,

$$(P_0 + \sqrt{D})/Q_0 = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{a_3 + \cdots}}}$$

We write $\langle a_0, a_1, a_2, \ldots \rangle$ for this continued fraction expansion. The a_i are the *partial quotients* of ξ_0.

Also, for $i \geq 0$, set $\xi_i = (P_i + \sqrt{D})/Q_i$ so the *conjugate* of ξ_i is $\overline{\xi_i} = (P_i - \sqrt{D})/Q_i$. Set $\xi = \xi_0$ and $\overline{\xi} = \overline{\xi_0}$. The ξ_i are the *i-th complete quotients* of ξ. These much-studied variables have many interesting properties, of which we list just a few.

- For $i > 0$, $a_i > 0$.
- Each of the sequences $\{a_i\}$, $\{P_i\}$, and $\{Q_i\}$ is eventually periodic. Specifically, there is a least nonnegative integer i_0 and

a least positive integer ℓ, the length of the minimal period, so that for any integers $i \geq i_0$ and $k > 0$, $a_{i+k\ell} = a_i$, $P_{i+k\ell} = P_i$, $Q_{i+k\ell} = Q_i$, and $\xi_{i+k\ell} = \xi_i$.

- For $i \geq i_0$, $0 < P_i < \sqrt{D}$, $0 < \sqrt{D} - P_i < Q_i < \sqrt{D} + P_i$, $Q_i \leq 2\left\lfloor \sqrt{D} \right\rfloor$.
- For $i \geq i_0$, if $Q_i \neq 1$ then $a_i < \sqrt{D}$, while if $Q_i = 1$ then $\sqrt{D} < a_i < 2\sqrt{D}$.
- For $i \geq i_0$, $\xi_i = (P_i + \sqrt{D})/Q_i$ is *reduced*, which means that $\xi_i > 1$ and $-1 < \overline{\xi_i} < 0$.
- $Q_i = Q_{i-2} - a_{i-1}(P_i - P_{i-1})$ for $i \geq 2$.
- $G_i = Q_0 A_i - P_0 B_i$ for $i \geq -2$.

3. Background

A *best approximation of the first kind* to a real number α is a rational number a/b with $b > 0$ so that if c/d is any other rational number with $0 < d \leq b$ then $|a/b - \alpha| < |c/d - \alpha|$.

In contrast, a *best approximation of the second kind* to a real number α is a rational number a/b with $b > 0$ so that if c/d is any other rational number with $0 < d \leq b$ then $|a - b\alpha| < |c - d\alpha|$. We will not discuss best approximations of the second kind beyond noting that a/b is a best approximation of the second kind to α if and only if a/b is a convergent to the continued fraction expansion of α.

If $a/b < c/d$ are rational numbers with $b > 0$ and $d > 0$, then their *mediant* is $(a + c)/(b + d)$ and it is not difficult to see that $a/b < (a + c)/(b + d) < c/d$, and similarly that for $j > 0$,

$$\frac{a}{b} < \frac{a + jc}{b + jd} < \frac{c}{d}.$$

By general properties of convergents to the continued fraction expansion of any irrational number α and mediants, we have the following inequalities:

$$(2)\quad \frac{A_0}{B_0} < \frac{A_1+A_0}{B_1+B_0} < \frac{2A_1+A_0}{2B_1+B_0} < \cdots < \frac{a_2A_1+A_0}{a_2B_1+B_0} = \frac{A_2}{B_2} < \frac{A_3+A_2}{B_3+B_2} < \frac{2A_3+A_2}{2B_3+B_2} < \cdots < \frac{a_4A_3+A_2}{a_4B_3+B_2} = \frac{A_4}{B_4} < \cdots < \alpha$$

$$(3)\quad \alpha < \cdots < \frac{A_5}{B_5} = \frac{a_5A_4+A_3}{a_5B_4+B_3} < \cdots < \frac{2A_4+A_3}{2B_4+B_3} < \frac{A_4+A_3}{B_4+B_3} < \frac{A_3}{B_3} = \frac{a_3A_2+A_1}{a_3B_2+B_1} < \cdots < \frac{2A_2+A_1}{2B_2+B_1} < \frac{A_2+A_1}{B_2+B_1} < \frac{A_1}{B_1}$$

The denominators satisfy the following inequalities:

$$(4)\quad B_0 \le B_1 < B_1+B_0 < 2B_1+B_0 < \cdots < a_2B_1+B_0 = B_2 < B_2+B_1 < 2B_2+B_1 < \cdots < a_3B_2+B_1 = B_3 < \cdots$$

The numerators satisfy corresponding inequalities, except that $A_0 < A_1$.

From the combination of equations (2), (3), and (4), we have that for $1 \le j < a_{i+1}$

$$\frac{jA_i + A_{i-1}}{jB_i + B_{i-1}}$$

is a best approximation to α if and only if

$$\left|\frac{jA_i + A_{i-1}}{jB_i + B_{i-1}} - \alpha\right| < \left|\frac{A_i}{B_i} - \alpha\right|$$

and that if

$$\frac{jA_i + A_{i-1}}{jB_i + B_{i-1}}$$

is a best approximation to α then

$$\frac{kA_i + A_{i-1}}{kB_i + B_{i-1}}$$

is a best approximation to α for all k such that $j \le k < a_{i+1}$.

4. Some best approximations to $\sqrt{D}$

We will show that if $\{t, u\}$ is any solution to $x^2 - Dy^2 = 1$, then for $0 \le j < \sqrt{D} - 1$

$$\frac{Du + jt}{t + ju}$$

is a best approximation of the first kind to $\sqrt{D}$ and is not a convergent to the continued fraction expansion of $\sqrt{D}$.

First note that if $t^2 - Du^2 = 1$ then $t = A_{k\ell-1}$ and $u = B_{k\ell-1}$ where ℓ is the length of the period of the continued fraction expansion of $\sqrt{D}$, $k\ell$ is even, and A_i/B_i are the convergents. For the partial quotients $(P_i + \sqrt{D})/Q_i$, we have $P_0 = 0$, $Q_0 = 1$, $P_{k\ell} = \lfloor\sqrt{D}\rfloor$, and $Q_{k\ell} = 1$. Formulas (16) and (17) of [3, p. 70] tell us that:

$$A_{i-1}Q_0 - B_{i-1}P_0 = B_{i-1}P_i + B_{i-2}Q_i$$

$$DB_{i-1} = (A_{i-1}P_i + A_{i-2}Q_i)Q_0 - (B_{i-1}P_i + B_{i-2}Q_i)P_0$$

Applying this with $i = k\ell$ to the continued fraction expansion of $\sqrt{D}$ gives us that

$$Du = \lfloor\sqrt{D}\rfloor A_{k\ell-1} + A_{k\ell-2}$$

and

$$t = \lfloor\sqrt{D}\rfloor B_{k\ell-1} + B_{k\ell-2}.$$

To show that Du/t is a best approximation all we have to do is show that

$$\left|\frac{Du}{t} - \sqrt{D}\right| < \left|\frac{t}{u} - \sqrt{D}\right|$$

First, because $t^2 - Du^2 = 1$, $t/u > \sqrt{D}$ and

$$\left|\frac{t}{u} - \sqrt{D}\right| = \frac{t}{u} - \sqrt{D}.$$

Also, $(Du)^2 - Dt^2 = D(Du^2 - t^2) = -D$ so $Du/t < \sqrt{D}$ and

$$\left|\frac{Du}{t} - \sqrt{D}\right| = \sqrt{D} - \frac{Du}{t}$$

Clearly

$$(t - u\sqrt{D})^2 > 0$$

so

$$t^2 - tu\sqrt{D} > tu\sqrt{D} - Du^2,$$

$$\left|\frac{t}{u}-\sqrt{D}\right|=\frac{t}{u}-\sqrt{D}>\sqrt{D}-\frac{Du}{t}=\left|\frac{Du}{t}-\sqrt{D}\right|$$

as was to be shown.

Similar arguments can be used to show that

$$\left|\frac{Du-t}{t-u}-\sqrt{D}\right|>\left|\frac{t}{u}-\sqrt{D}\right|$$

When $t^2-Du^2=-1$, similar arguments can be used to show that

$$\left|\frac{Du}{t}-\sqrt{D}\right|>\left|\frac{t}{u}-\sqrt{D}\right|$$

and

$$\left|\frac{Du+t}{t+u}-\sqrt{D}\right|<\left|\frac{t}{u}-\sqrt{D}\right|$$

which is sufficient to establish our claims that the fractions listed are best approximations when $t^2-Du^2=-1$.

The best approximations considered above are not convergents because

$$t=aB_{j\ell-1}+B_{j\ell-2}$$

for $a=\left\lfloor\sqrt{D}\right\rfloor$ and some $j>0$, and so

$$B_{j\ell-1}<mB_{j\ell-1}+B_{j\ell-2}<B_{j\ell}$$

when $a\le m<2a=a_{j\ell}$. So the denominators of these best approximations are not denominators of convergents.

Here's an example of a best approximation of the first kind to $\sqrt{1105}$ that is not a convergent or based on a solution to $x^2-1105y^2=\pm1$. For $\sqrt{1105}$, $\ell=5$, $A_1=133$, $A_0=33$, $B_1=4$, and $B_0=1$. We have that $565/17=(4\cdot 133+33)/(4\cdot 4+1)$ is a best approximation that is clearly not of the form $(kA_{5j-1}+A_{5j-2})/(kB_{5j-1}+B_{5j-2})$ for any $j\ge 0$ and any k with $0\le k<a_{5j}$.

5. A property of best approximations

We prove that if a/b is a best approximation to $\sqrt{D}$ then $|a^2-Db^2|\le D$.

By the above, any best approximation is

$$\frac{rA_i+A_{i-1}}{rB_i+B_{i-1}}$$

for some $0 \leq r < a_{i+1}$

We have

$$(5)\quad (rA_i + A_{i-1})^2 - D(rB_i + B_{i-1})^2$$
$$= r^2(A_i^2 - DB_i^2) + 2r(A_iA_{i-1} - DB_iB_{i-1}) + A_{i-1}^2 - DB_{i-1}^2$$
$$= r^2Q_{i+1}(-1)^{i+1} + 2rP_{i+1}(-1)^i + Q_i(-1)^i$$
$$= (-1)^{i+1}(r^2Q_{i+1} - 2rP_{i+1} - Q_i)$$

where

$$A_iA_{i-1} - DB_iB_{i-1} = P_{i+1}(-1)^i$$

is easily established by induction.

The derivative with respect to r of the quadratic polynomial

$$(6)\qquad f(r) = r^2Q_{i+1} - 2rP_{i+1} - Q_i,$$

which appears in the last line of (5), is

$$f'(r) = 2rQ_{i+1} - 2P_{i+1}.$$

Hence the minimum value for f(r) occurs at $r = P_{i+1}/Q_{i+1}$ and is $f(P_{i+1}/Q_{i+1}) = \frac{P_{i+1}^2}{Q_{i+1}} + Q_i$. Note that

$$0 < \frac{P_{i+1}}{Q_{i+1}} < a_{i+1}.$$

To see that $|rA_i + A_{i-1})^2 - D(rB_i + B_{i-1})^2| \leq D$, for $0 \leq r \leq a_{i+1}$, it suffices to verify this for $r = 0$, $r = a_{i+1}$, and $r = P_{i+1}/Q_{i+1}$ (the endpoints of the interval of interest and point where the quadratic function takes its minimum value).

If $r = 0$, then $|f(r)| = |Q_i| \leq 2\left\lfloor \sqrt{D} \right\rfloor \leq D$.

If $r = a_{i+1}$, then $rA_i + A_{i-1} = A_{i+1}$ and $rB_i + B_{i-1} = B_{i+1}$, so

$$f(r) = A_{i+1}^2 - DB_{i+1}^2 = (-1)^{i+2}Q_{i+2}.$$

Whence $|f(r)| = |Q_{i+2}| \leq 2\left\lfloor \sqrt{D} \right\rfloor \leq D$.

At $r = P_{i+1}/Q_{i+1}$,

$$|f(r)| = |r^2Q_{i+1} - 2rP_{i+1} - Q_i| = \frac{P_{i+1}^2}{Q_{i+1}} + Q_i.$$

But we have

$$D \leq DQ_{i+1},$$

so

$$P_{i+1}^2 + \{D - P_{i+1}^2\} \le DQ_{i+1},$$

so

$$P_{i+1}^2 + Q_i Q_{i+1} \le DQ_{i+1},$$

so

$$\frac{P_{i+1}^2}{Q_{i+1}} + Q_i \le D$$

which is all we need to complete the proof.

Note that equality occurs if and only if $Q_{i+1} = 1$.

References

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