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MIDPOINT CRITERIA FOR SOLVING PELL'S EQUATION USING THE NEAREST SQUARE CONTINUED FRACTION

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ABSTRACT. We derive midpoint criteria for Pell's equation $x^2 - Dy^2 = \pm 1$, using the nearest square continued fraction expansion of $\sqrt{D}$. The period of the expansion is on average 70% that of the regular continued fraction. We also derive similar criteria for the diophantine equation $x^2 - xy - \frac{(D-1)}{4}y^2 = \pm 1$, where $D \equiv 1 \pmod 4$. We also present some numerical results and conclude with a comparison of the computational performance of the regular, nearest square and nearest integer continued fraction algorithms.

1. Introduction

Euler gave two *midpoint* criteria for solving Pell's equation $x^2 - Dy^2 = \pm 1$ using the regular continued fraction (RCF) expansion of $\sqrt{D}$ (see [4, p. 358]). Suppose the simple continued fraction expansion for $\sqrt{D}$ is periodic with period k:

$$\sqrt{D} = \begin{cases} [a_0, \overline{a_1, \ldots, a_{h-1}, a_{h-1}, \ldots, a_1, 2a_0}] & \text{if } k = 2h-1, \\ [a_0, \overline{a_1, \ldots, a_{h-1}, a_h, a_{h-1}, \ldots, a_1, 2a_0}] & \text{if } k = 2h. \end{cases}$$

Then the smallest solution of $x^2 - Dy^2 = \pm 1$ is given by

$$\eta = A_{k-1} + B_{k-1}\sqrt{D},$$

where A_n/B_n is the n-th convergent to $\sqrt{D}$. Euler observed that if $k = 2h-1$,

$$\begin{aligned} A_{2h-2} &= A_{h-1}B_{h-1} + A_{h-2}B_{h-2} \\ B_{2h-2} &= B_{h-1}^2 + B_{h-2}^2, \end{aligned}$$

while if $k = 2h$,

$$\begin{aligned} A_{2h-1} &= A_{h-1}B_h + A_{h-2}B_{h-1} \\ B_{2h-1} &= B_{h-1}(B_h + B_{h-2}). \end{aligned}$$

Also if $(P_n + \sqrt{D})/Q_n$ denotes the n-th complete quotient of the RCF expansion of $\sqrt{D}$, if $Q_h = Q_{h-1}$ then $k = 2h-1$; while if $P_h = P_{h+1}$, then $k = 2h$. Consequently we can detect the end of the half period.

H.C. Williams and P.A. Buhr [13] gave six midpoint criteria for the *nearest integer* continued fraction of B. Minnegerode [7] and A. Hurwitz [5]. In our paper, we give three midpoint criteria in terms of the *nearest square* continued fraction.

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2. Nearest square continued fraction

This continued fraction was introduced by A.A.K. Ayyangar in 1940 and 1941 (see [2], [3]) and arose from Bhaskara's cyclic method (1150) for solving Pell's equation (see [1]). Let $\xi_0 = \frac{P+\sqrt{D}}{Q}$ be a surd in *standard form*, i.e., D is a non-square positive integer and $P, Q \neq 0, \frac{D-P^2}{Q}$ are integers, having no common factor other than 1. Then with $c = \lfloor \xi_0 \rfloor$, the integer part of ξ_0, we can represent ξ_0 in one of two forms

$$\xi_0 = c + \frac{Q'}{P' + \sqrt{D}} \qquad \text{or } \xi_0 = c + 1 - \frac{Q''}{P'' + \sqrt{D}},$$

where $\frac{P'+\sqrt{D}}{Q'} > 1$ and $\frac{P''+\sqrt{D}}{Q''} > 1$ are also standard surds. We choose the partial denominator a_0 and numerator ϵ_1 of the new continued fraction development as follows:

(a) $a_0 = c$ if $|Q'| < |Q''|$, or $|Q'| = |Q''|$ and $Q < 0$, $\epsilon_1 = 1$,
(b) $a_0 = c + 1$ if $|Q'| > |Q''|$, or $|Q'| = |Q''|$ and $Q > 0$, $\epsilon_1 = -1$.

The term *nearest square* arises on restating (a) and (b):

(a′) $a_0 = c$ if $|P'^2 - D| < |P''^2 - D|$, or $|P'^2 - D| = |P''^2 - D|$ and $Q < 0$,
(b′) $a_0 = c + 1$ if $|P'^2 - D| > |P''^2 - D|$, or $|P'^2 - D| = |P''^2 - D|$ and $Q > 0$.

Then $\xi_0 = a_0 + \frac{\epsilon_1}{\xi_1}$, where $|\epsilon_1| = 1, a_0$ an integer and $\xi_1 = \frac{P_1+\sqrt{D}}{Q_1} > 1$. Also $P_1 = P'$ or P'' and $Q_1 = Q'$ or Q'', according as $\epsilon_1 = 1$ or -1. We proceed similarly with ξ_1 and so on. Then

$$\xi_n = a_n + \frac{\epsilon_{n+1}|}{|\xi_{n+1}} \text{ and } \xi_0 = a_0 + \frac{\epsilon_1|}{|a_1} + \frac{\epsilon_2|}{|a_2} + \cdots \tag{2.1}$$

This development is called the *nearest square continued fraction* (NSCF).

Analogous relations to those for regular continued fractions, hold for P_n, Q_n and a_n:

$$P_{n+1} + P_n = a_n Q_n \tag{2.2}$$

$$P_{n+1}^2 + \epsilon_{n+1} Q_n Q_{n+1} = D. \tag{2.3}$$

By Theorem I (iii)[3, p. 22], the $|Q_n|$ successively diminish as long as $|Q_n| > \sqrt{D}$ and so ultimately, we have $|Q_n| < \sqrt{D}$. When this stage is reached, the P_m and Q_m thereafter become positive and bounded, $0 < P_m < 2\sqrt{D}, 0 < Q_m < \sqrt{D}$ by Theorem I (iv)[3, p. 22]. This implies eventual periodicity of the complete quotients and thence the partial quotients. In particular, Theorem XII ([3, pp. 102-103]) shows that the NSCF development of $\sqrt{D}$ has the form

$$\sqrt{D} = a_0 + \frac{\epsilon_1|}{|\overset{*}{a_1}} + \cdots + \frac{\epsilon_k|}{|\overset{*}{2a_0}}, \tag{2.4}$$

where the asterisks denote that the period-length is k and $\xi_p = \xi_{p+k}$, $\epsilon_p = \epsilon_{p+k}$ and $a_p = a_{p+k}$ for $p \geq 1$. (It's an easy exercise to show that $a_0 = [\sqrt{D}]$, the nearest integer to $\sqrt{D}$.) In [3, pp. 112-114], the finer structure of (2.4) is revealed. There are two types:

Type I: No complete quotient of a cycle has the form $\frac{p+q+\sqrt{p^2+q^2}}{p}$, where $p > 2q > 0$, $\gcd(p, q) = 1$. This type possesses the classical symmetries of the regular continued fraction if $k > 1$:

$$\begin{array}{rcrl} a_v & = & a_{k-v}, & 1 \le v \le k-1, \\ Q_v & = & Q_{k-v}, & 1 \le v \le k-1, \\ \epsilon_v & = & \epsilon_{k+1-v}, & 1 \le v \le k, \\ P_v & = & P_{k+1-v}, & 1 \le v \le k. \end{array}$$

For example, $\sqrt{19} = 4 + \frac{1|}{\underset{*}{|3}} - \frac{1|}{|5} - \frac{1|}{|3} + \frac{1|}{\underset{*}{|8}}$.

Type II: One complete quotient ξ_v in a cycle has the form $\frac{p+q+\sqrt{p^2+q^2}}{p}$, where $p > 2q > 0$. In this case $k \ge 4$ is even and $v = k/2$. This type also possesses the symmetries of Type I, apart from

$$a_{\frac{k}{2}} = 2, \epsilon_{\frac{k}{2}} = -1, \epsilon_{\frac{k}{2}+1} = 1, a_{\frac{k}{2}-1} = a_{\frac{k}{2}+1} + 1, P_{\frac{k}{2}} \ne P_{\frac{k}{2}+1}$$

and we have

$$\sqrt{D} = a_0 + \frac{\epsilon_1|}{\underset{*}{|a_1}} + \cdots + \frac{\epsilon_{\frac{k}{2}-1}|}{|a_{\frac{k}{2}-1}} - \frac{1|}{|2} + \frac{1|}{|a_{\frac{k}{2}-1} - 1} + \cdots + \frac{\epsilon_k|}{\underset{*}{|2a_0}}. \tag{2.5}$$

For example, $\sqrt{29} = 5 + \frac{1|}{\underset{*}{|3}} - \frac{1|}{|2} + \frac{1|}{|2} + \frac{1|}{\underset{*}{|10}}$. Other examples are $D = 53, 58, 85, 97$.

For both types of D, we have $Q_k = 1$. For $P_1 = a_0$, $P_1 = P_k$ (symmetry), $P_1 = P_{k+1}$, (periodicity), so

$$\begin{aligned} 2a_0 = 2P_1 = P_k + P_{k+1} &= a_k Q_k \text{ by (2.2)}, \\ &= 2a_0 Q_k. \end{aligned}$$

Hence $Q_k = 1$ and $\xi_k = a_0 + \sqrt{D}$. This is needed later in the proof of Lemma 1.

Similarly, the quadratic surd $\xi_0 = (1 + \sqrt{D})/2$, $D = 4n + 1$, has $a_0 = [\xi_0]$. Also $a_k = 2a_0 - 1 = P_1$ and

$$2P_1 = P_k + P_{k+1} = a_k Q_k = P_1 Q_k.$$

Hence $Q_k = 2$ and $\xi_k = (2a_0 - 1 + \sqrt{D})/2$.

3. Reduced NSCF quadratic surds

Ayyangar [3, p. 27] gives a definition of reduced quadratic surd that is not as explicit as for regular continued fractions (see e.g. [8, p. 73]). He defines a *special* surd ξ_v by the inequalities

$$Q_{v-1}^2 + \tfrac{1}{4}Q_v^2 \le D, \quad Q_v^2 + \tfrac{1}{4}Q_{v-1}^2 \le D \tag{3.1}$$

then defines a *semi-reduced* surd to be the successor of a special surd. Finally a *reduced* surd to defined to be the successor of a semi-reduced surd. He proves ([3, p. 28]) that a reduced surd is a special surd and in ([3, p. 101-102]) that a quadratic surd has a purely periodic NSCF if and only if it is reduced. Examples of reduced surds that figure prominently in [3] are (i) $\frac{p+q+\sqrt{p^2+q^2}}{p}$, where $p > 2q > 0$ and (ii) the successor of $\sqrt{D}$.

4. Midpoint properties of Types I and II NSCF expansions of $\sqrt{D}$

(a) Type I: If $k = 2h$, then $P_h = P_{h+1}$.
(b) Type I: If $k = 2h + 1$, then $Q_h = Q_{h+1}$.
(c) Type II: Here $k = 2h$, Q_{h-1} is even, $\epsilon_h = -1$ and $P_h = Q_h + \frac{1}{2}Q_{h-1}$. Also $P_v \neq P_{v+1}$ and $Q_v \neq Q_{v+1}$ for $1 \leq v < 2h$.

(See [3, pp. 110-114].) There are converses: Assume $k > 1$ and $1 \leq v < k$. Then

(d) $P_v = P_{v+1} \implies k = 2h$, $v = h$ and a Type I NSCF expansion.
(e) $Q_v = Q_{v+1} \implies k = 2h + 1$, $v = h$ and a Type I NSCF expansion.
(f) Q_{v-1} even, $\epsilon_v = -1$ and $P_v = Q_v + \frac{1}{2}Q_{v-1} \implies k = 2h, v = h$ and a Type II NSCF expansion.

Proof. (d) is proved in [3, p. 111]: Suppose $P_v = P_{v+1}$. Then we know we are dealing with a Type I NSCF expansion and hence $Q_{k-v} = Q_v$. Then

$$\xi_{k-v} = \frac{P_{k-v} + \sqrt{D}}{Q_{k-v}} = \frac{P_{v+1} + \sqrt{D}}{Q_v} = \frac{P_v + \sqrt{D}}{Q_v} = \xi_v,$$

so $k - v = v$ and $k = 2v$.

(e) is similar.

(f) Assume Q_{v-1} even, $\epsilon_v = -1$ and $P_v = Q_v + \frac{1}{2}Q_{v-1}$. Then

$$\begin{aligned} D = P_v^2 + \epsilon_v Q_v Q_{v-1} &= P_v^2 - Q_v Q_{v-1} \\ &= (Q_v + \tfrac{1}{2}Q_{v-1})^2 - Q_v Q_{v-1} \\ &= Q_v^2 + \tfrac{1}{4}Q_{v-1}^2 \\ &= p^2 + q^2, \end{aligned}$$

where $p = Q_v, q = \frac{1}{2}Q_{v-1}$. Also $\gcd(p, q) = 1$. Next, because ξ_v is reduced, it is a special surd ([3, p. 27]), so $Q_{v-1}^2 + \frac{1}{4}Q_v^2 \leq D$. Hence

$$\begin{aligned} Q_{v-1}^2 + \tfrac{1}{4}Q_v^2 &\leq Q_v^2 + \tfrac{1}{4}Q_{v-1}^2, \\ \tfrac{3}{4}Q_{v-1}^2 &\leq \tfrac{3}{4}Q_v^2, \\ Q_{v-1} &\leq Q_v. \end{aligned}$$

But $Q_v = Q_{v-1}$ implies $p = 2q$, so $p = 2, q = 1, D = 5$ and $\xi_v = \frac{3+\sqrt{5}}{2}$. However this implies $k = 1$, so we deduce $p > 2q$ and ξ_v has the form $\frac{p+q+\sqrt{D}}{p}$, where $p > 2q > 0$. Hence we are dealing with a Type II NSCF expansion with $k = 2h$ and $v = h$. □

5. The convergents and Pell's equation

As in [12, p. 406], we define the *convergents* A_n/B_n by $A_{-2} = 0, A_{-1} = 1, B_{-2} = 1, B_{-1} = 0$ and for $i \geq -1$,

$$\begin{aligned} A_{i+1} &= a_{i+1}A_i + \epsilon_{i+1}A_{i-1} \\ B_{i+1} &= a_{i+1}B_i + \epsilon_{i+1}B_{i-1}. \end{aligned}$$

An important property of the convergents to $\xi_0 = \frac{P_0+\sqrt{D}}{Q_0}$ is

$$(Q_0A_n - P_0B_n)^2 - DB_n^2 = (-1)^{n+1}\epsilon_1\epsilon_2 \cdots \epsilon_{n+1}Q_{n+1}. \tag{5.1}$$

(see [12, (3.3) p. 406 and (3.5) p. 407].) For $\xi_0 = \sqrt{D}$, this reduces to

$$A_n^2 - DB_n^2 = (-1)^{n+1}\epsilon_1\epsilon_2 \cdots \epsilon_{n+1}Q_{n+1}. \tag{5.2}$$

Hence, as $Q_k = 1$, we have

$$A_{k-1}^2 - DB_{k-1}^2 = (-1)^k \epsilon_1\epsilon_2\cdots\epsilon_k. \tag{5.3}$$

Remark. Similarly, from (5.1), the convergents to $(1+\sqrt{D})/2, D \equiv 1 \pmod 4$ satisfy

$$A_n^2 - A_nB_n - \frac{(D-1)}{4}B_n^2 = (-1)^{n+1}\epsilon_1\epsilon_2\cdots\epsilon_{n+1}Q_{n+1}/2. \tag{5.4}$$

Hence, as $Q_k = 2$, we have

$$A_{k-1}^2 - A_{k-1}B_{k-1} - \frac{(D-1)}{4}B_{k-1}^2 = (-1)^k\epsilon_1\epsilon_2\cdots\epsilon_k. \tag{5.5}$$

Lemma 1. *In the NSCF expansion of $\sqrt{D}$, with period-length k, $Q_n = 1$ if and only if k divides n.*

Proof. We have seen that $Q_k = 1$. So suppose $Q_n = 1, n \geq 1$. Then from (2.3), $P_n^2 + \epsilon_n Q_{n-1} = D$.

Case 1. $P_n > \sqrt{D}$. Then $\epsilon_n = -1$. Hence

$$P_n^2 - D = Q_{n-1} < \sqrt{D} \ (\xi_n \text{ is reduced})$$

$$0 < P_n - \sqrt{D} < \frac{\sqrt{D}}{P_n + \sqrt{D}} < \frac{\sqrt{D}}{2\sqrt{D}} = \frac{1}{2}.$$

Hence $P_n = [\sqrt{D}]$.

Case 2. $P_n < \sqrt{D}$. Then $\epsilon_n = 1$. Hence

$$\begin{aligned} Q_{n-1}^2 + \tfrac{1}{4}Q_n^2 &\leq D = P_n^2 + Q_{n-1} \ (\xi_n \text{ is reduced}) \\ (Q_{n-1} - \tfrac{1}{2})^2 &\leq P_n^2 \\ Q_{n-1} - \tfrac{1}{2} &\leq P_n \\ Q_{n-1} &\leq P_n + \tfrac{1}{2} \\ D - P_n^2 = Q_{n-1} &\leq P_n. \end{aligned}$$

Hence $0 < \sqrt{D} - P_n \leq \frac{P_n}{\sqrt{D}+P_n} < \frac{P_n}{2P_n} = \frac{1}{2}$ and again $P_n = [\sqrt{D}]$.

Thus in both cases, $\xi_n = a_0 + \sqrt{D} = \xi_k$ and k divides n. □

In the next section we prove that there is no smaller positive integer solution (x, y) of the equation $x^2 - Dy^2 = \pm 1$ than (A_{k-1}, B_{k-1}) by showing that x/y is a convergent in the NSCF expansion of $\sqrt{D}$.

Remark. Similarly, in the NSCF expansion of $(1+\sqrt{D})/2, D \equiv 1 \pmod 4$, with period-length k, $Q_n = 2$ if and only if k divides n.

6. Relations between the NSCF and RCF

In [8, pp. 147-155], Perron introduces a transformation $\mathfrak{t}_1$ of the following NSCF (with trivial modification when $\lambda = 0$):

$$\xi_0 = a_0 + \frac{\epsilon_1}{|a_1} + \cdots + \frac{\epsilon_\lambda}{|a_\lambda} - \frac{1}{|a_{\lambda+1}} + \frac{\epsilon_{\lambda+2}}{|a_{\lambda+2}} + \cdots \tag{6.1}$$

expanding it to

$$\xi_0 = a_0 + \frac{\epsilon_1|}{|a_1} + \cdots + \frac{\epsilon_\lambda|}{|a_\lambda - 1} + \frac{1|}{|1} + \frac{1|}{|a_{\lambda+1} - 1} + \frac{\epsilon_{\lambda+2}|}{|a_{\lambda+2}} + \cdots \tag{6.2}$$

The overall result of applying $\mathfrak{t}_1$ at all occurrences of $\epsilon_\lambda = -1$ is a transformation $\mathfrak{T}_1$, given by the rule: Before a negative partial numerator the term $\frac{+1|}{|1}$ is inserted. Also each a_ν is replaced by

(a) a_ν if $\epsilon_\nu = +1$, $\epsilon_{\nu+1} = +1$,
(b) $a_\nu - 1$ if $\epsilon_\nu = +1$, $\epsilon_{\nu+1} =$ -1, or $\epsilon_\nu =$ -1, $\epsilon_{\nu+1} = +1$,
(c) $a_\nu - 2$ if $\epsilon_\nu =$ -1, $\epsilon_{\nu+1} =$ -1.

Here $\epsilon_0 = +1$.

The partial quotients corresponding to a NSCF reduced quadratic surd are greater than 1 ([3, p. 29]). So in view of Lemma 2 below and (b) and (c) above, $\mathfrak{T}_1$ will convert the NSCF expansion of $\sqrt{D}$ into a RCF expansion.

Lemma 2. *Suppose ξ_v and ξ_{v-1} are NSCF reduced quadratic surds. Then if $\epsilon_v = -1$ and $\epsilon_{v+1} = -1$, we have $a_v \geq 3$.*

Proof. Assume ξ_v and ξ_{v-1} are reduced. Then from [3, p. 27], we have

$$P_{v+1} \geq Q_v + \tfrac{1}{2}Q_{v+1} \tag{6.3}$$

$$P_v \geq Q_v + \tfrac{1}{2}Q_{v-1}. \tag{6.4}$$

Then (6.3) and (6.4) give

$$a_v Q_v = P_{v+1} + P_v \geq 2Q_v + \tfrac{1}{2}Q_{v+1} + \tfrac{1}{2}Q_{v-1}.$$

Hence $a_v Q_v > 2Q_v$, as $Q_{v+1} > 0$ and $Q_{v-1} > 0$. Hence $a_v > 2$. □

Lemma 3. *The period length of the RCF expansion of $\sqrt{D}$ is $k + r$, where r is the number of $\epsilon_\nu = -1$ occurring in the period partial numerators $\epsilon_1, \ldots, \epsilon_k$ of the NSCF expansion of $\sqrt{D}$.*

Proof. If $r = 0$, there is nothing to prove. So we assume $r > 0$. According to [8, Satz 5.9, p. 152], under $\mathfrak{T}_1$,

(i) $\epsilon_{\nu+1} = -1$ gives rise to RCF convergents

$$A'_{m-1}/B'_{m-1} = (A_\nu - A_{\nu-1})/(B_\nu - B_{\nu-1}), \quad A'_m/B'_m = A_\nu/B_\nu$$

and RCF complete quotients

$$\frac{P'_m + \sqrt{D}}{Q'_m} = \xi_{\nu+1}/(\xi_{\nu+1} - 1), \quad \frac{P'_{m+1} + \sqrt{D}}{Q'_{m+1}} = \xi_{\nu+1} - 1.$$

(ii) $\epsilon_{\nu+1} = 1$ gives rise to RCF convergent A_ν/B_ν and RCF complete quotient $\xi_{\nu+1}$.

Consequently the NSCF complete quotients $\xi_1, \ldots, \xi_k$ will give rise to a RCF period $\xi'_1, \ldots, \xi'_{k+r}$ of complete quotients. We prove that this is a least period.

This will follow by showing that $\xi_i/(\xi_i - 1) = a + \sqrt{D}$ is impossible. For $a + \sqrt{D}$ is RCF-reduced and hence $a = \lfloor\sqrt{D}\rfloor$. We can assume $D > 3$. Then $a > 1$ and

$$\xi_i = \frac{a+\sqrt{D}}{a-1+\sqrt{D}} = 1 + \frac{1}{a-1+\sqrt{D}} = 2 - \frac{a-2+\sqrt{D}}{a-1+\sqrt{D}} \tag{6.5}$$

$$= 2 - \frac{D-(a-2)^2}{D-(a-1)(a-2)+\sqrt{D}}. \tag{6.6}$$

Then $Q''_{i+1} = D-(a-2)^2 = D-a^2+4(a-1) > 1 = Q'_{i+1}$.

Hence (6.5) is the NSCF expansion of ξ_i. But partial denominators of such a reduced surd are at least 2 (see [3, Corollary 4, p. 29]), so we have a contradiction.

So under $\mathfrak{T}_1$, the NSCF complete quotients $\xi_1, \ldots, \xi_k$ will produce a period of RCF complete quotients $\xi'_m = \frac{P'_m+\sqrt{D}}{Q'_m}, 1 \leq m \leq k+r$, where $Q'_m > 1$ if $1 \leq m < k+r$ and $Q'_{k+r} = 1$. Consequently this is a least period of the RCF expansion of $\sqrt{D}$. □

Lemma 4. *If $x^2 - Dy^2 = \pm 1$, $x, y > 0$, then x/y is a NSCF convergent to $\sqrt{D}$.*

Proof. For x/y is a RCF convergent A'_{m-1}/B'_{m-1} to $\sqrt{D}$, so

$$A'^2_{m-1} - DB'^2_{m-1} = (-1)^m Q'_m = (-1)^m.$$

If x/y is not a NSCF convergent of $\sqrt{D}$, it has the form $(A_n - A_{n-1})/(B_n - B_{n-1})$, where $\epsilon_{n+1} = -1$. However this would imply $\xi_{n+1}/(\xi_{n+1}-1) = \frac{P'_m+\sqrt{D}}{Q'_m}$ and we have seen that this is impossible. Hence x/y is a NSCF convergent to $\sqrt{D}$. □

Remark. The diophantine equation $x^2 - xy - \frac{(D-1)}{4}y^2 = \pm 1, D \equiv 1 \pmod 4$ is also of interest. We can similarly show that if $D \geq 13$ and $x > 0, y > 0$, then x/y is a NSCF convergent to $(1+\sqrt{D})/2$.

7. Midpoint criteria for determining A_{k-1} and B_{k-1}

Exactly one of the following will apply for any $D > 0$, not a square:

P-test: : For some h, $1 \leq h < k$, $P_h = P_{h+1}$, in which case $k = 2h$ and

$$A_{k-1} = A_h B_{h-1} + \epsilon_h A_{h-1} B_{h-2} \tag{7.1}$$

$$B_{k-1} = B_{h-1}(B_h + \epsilon_h B_{h-2}). \tag{7.2}$$

In this case $A^2_{k-1} - DB^2_{k-1} = 1$.

Q-test: : For some h, $0 \leq h < k$, $Q_h = Q_{h+1}$, in which case $k = 2h+1$ and

$$A_{k-1} = A_h B_h + \epsilon_{h+1} A_{h-1} B_{h-1} \tag{7.3}$$

$$B_{k-1} = B_h^2 + \epsilon_{h+1} B^2_{h-1}. \tag{7.4}$$

In this case $A^2_{k-1} - DB^2_{k-1} = -\epsilon_{h+1}$.

PQ-test: : For some h, $1 \leq h < k$, Q_{h-1} is even, $P_h = Q_h + \frac{1}{2}Q_{h-1}$ and $\epsilon_h = -1$, in which case $k = 2h$ and

$$A_{k-1} = A_h B_{h-1} - B_{h-2}(A_{h-1} - A_{h-2}) \tag{7.5}$$

$$B_{k-1} = 2B^2_{h-1} - B_h B_{h-2}. \tag{7.6}$$

In this case $A^2_{k-1} - DB^2_{k-1} = -1$.

Before we prove these statements, we restate the symmetry properties of the partial numerators and denominators of the NSCF expansion of $\sqrt{D}$ in the following form, for use in Lemma 5 below:

(1) If $k = 2h + 1$ and $1 \le t \le h$, then

$$\epsilon_{h+1+t} = \epsilon_{h+1-t} \tag{7.7}$$

$$a_{h+t} = a_{h+1-t}, \tag{7.8}$$

(2) If $k = 2h$ and Type I with $1 \le t \le h$ or Type II with $3 \le t \le h$, then

$$\epsilon_{h+t} = \epsilon_{h-t+1} \tag{7.9}$$

$$a_{h+t-1} = a_{h-t+1}, \tag{7.10}$$

Lemma 5. (i) *Let $k = 2h+1, h \ge 1$. Then for Type I and $0 \le t \le h$, we have*

$$A_{2h} = A_{h+t}B_{h-t} + \epsilon_{h+1+t}A_{h+t-1}B_{h-t-1} \tag{7.11}$$

$$B_{2h} = B_{h+t}B_{h-t} + \epsilon_{h+1+t}B_{h+t-1}B_{h-t-1} \tag{7.12}$$

(ii) *Let $k = 2h, h \ge 1$. Then for Type I and $0 \le t \le h$, or Type II with $h \ge 2$ and $2 \le t \le h$, we have*

$$A_{2h-1} = A_{h+t-1}B_{h-t} + \epsilon_{h+t}A_{h+t-2}B_{h-t-1} \tag{7.13}$$

$$B_{2h-1} = B_{h+t-1}B_{h-t} + \epsilon_{h+t}B_{h+t-2}B_{h-t-1} \tag{7.14}$$

Proof. We prove (7.11) by induction on t, $h \ge t \ge 0$. Let

$$f(t) = A_{h+t}B_{h-t} + \epsilon_{h+1+t}A_{h+t-1}B_{h-t-1}.$$

We show $f(h) = A_{2h}$ and $f(t) = f(t-1)$ if $h \ge t \ge 1$.

First note that (7.11) holds when $t = h$. For then

$$f(h) = A_{2h}B_0 + \epsilon_{2h+1}A_{2h-1}B_{-1} = A_{2h}.$$

Next

$$\begin{aligned} f(t) &= A_{h+t}B_{h-t} + \epsilon_{h+1+t}A_{h+t-1}B_{h-t-1} \\ &= (a_{h+t}A_{h+t-1} + \epsilon_{h+t}A_{h+t-2}) + \epsilon_{h+1+t}A_{h+t-1}B_{h-t-1} \\ &= A_{h+t-1}(a_{h+t}B_{h-t} + \epsilon_{h+1+t}B_{h-t-1}) + \epsilon_{h+t}A_{h+t-2}B_{h-t} \\ &= A_{h+t-1}(a_{h+1-t}B_{h-t} + \epsilon_{h+1-t}B_{h-t-1}) + \epsilon_{h+t}A_{h+t-2}B_{h-t} \\ &= A_{h+t-1}B_{h+1-t} + \epsilon_{h+t}A_{h+t-2}B_{h-t} = f(t-1). \end{aligned}$$

Similarly for equation (7.12).

Equations (7.13) and (7.14) are proved similarly using equations (7.9) and (7.10), noting that for Type II, we can assume $h \ge 3$, for if $h = 2$, equations (7.13) and (7.14) are trivially true. □

The P**-test**: Substituting $t = 0$ in (7.13) gives

$$\begin{aligned} A_{2h-1} &= A_{h-1}B_h + \epsilon_h A_{h-2}B_{h-1} \\ &= A_{h-1}(a_hB_{h-1} + \epsilon_hB_{h-2}) + (A_h - a_hA_{h-1})B_{h-1} \\ &= A_hB_{h-1} + \epsilon_hA_{h-1}B_{h-2}, \end{aligned}$$

which is the first equation of the P-test. Substituting $t = 0$ in (7.14) gives

$$B_{2h-1} = B_{h-1}B_h + \epsilon_hB_{h-2}B_{h-1},$$

which is the second equation of the P-test.

The **Q-test**: If $k = 1$, then equations (7.3) and (7.4) are trivially true. So we can assume $k > 1$. Then substituting $t = 0$ in (7.11) gives

$$A_{2h} = A_h B_h + \epsilon_{h+1} A_{h-1} B_{h-1},$$

which is the first equation in the Q-test. Substituting $t = 0$ in (7.12) gives

$$B_{2h} = B_h B_h + \epsilon_{h+1} B_{h-1} B_{h-1},$$

which is the second equation of the Q-test.

The **PQ-test**: We take $t = 2$ in equations (7.13) and (7.14) to get

$$A_{2h-1} = A_{h+1} B_{h-2} + \epsilon_{h+2} A_h B_{h-3} \tag{7.15}$$

$$B_{2h-1} = B_{h+1} B_{h-2} + \epsilon_{h+2} B_h B_{h-3}. \tag{7.16}$$

We also have

$$\epsilon_h = -1, \epsilon_{h+1} = 1, a_{h+1} = a_{h-1} - 1, a_h = 2, \epsilon_{h+2} = \epsilon_{h-1}. \tag{7.17}$$

Also $B_{h-1} = a_{h-1} B_{h-2} + \epsilon_{h-1} B_{h-3}$. Hence (7.15) gives

$$\begin{aligned} A_{2h-1} &= (a_{h+1} A_h + \epsilon_{h+1} A_{h-1}) B_{h-2} + \epsilon_{h-1} A_h B_{h-3} \\ &= (a_{h+1} A_h + \epsilon_{h+1} A_{h-1}) B_{h-2} + (B_{h-1} - a_{h-1}) A_h \\ &= (a_{h+1} - a_h) A_h B_{h-2} + A_{h-1} B_{h-2} + B_{h-1} A_h \\ &= -A_h B_{h-2} + A_{h-1} B_{h-2} + B_{h-1} A_h \\ &= B_{h-1} A_h - (A_h - A_{h-1}) B_{h-2}. \qquad (7.18) \end{aligned}$$

But $A_h = a_h A_{h-1} + \epsilon_h A_{h-2} = 2A_{h-1} - A_{h-2}$. Hence

$$A_h - A_{h-1} = A_{h-1} - A_{h-2}$$

and (7.18) gives

$$A_{2h-1} = A_h B_{h-1} - (A_{h-1} - A_{h-2}) B_{h-2},$$

which is the first equation of the PQ-test. Finally, (7.16) gives

$$\begin{aligned} B_{2h-1} &= (a_{h+1} B_h + \epsilon_{h+1} B_{h-1}) B_{h-2} + \epsilon_{h-1} B_h B_{h-3} \\ &= (a_{h+1} B_h + \epsilon_{h+1} B_{h-1}) B_{h-2} + B_h (B_{h-1} - a_{h-1} B_{h-2}) \\ &= (a_{h+1} - a_{h-1}) B_h B_{h-2} + B_{h-1} (\epsilon_{h+1} B_{h-2} + B_h) \\ &= -B_h B_{h-2} + B_{h-1} (B_{h-2} + B_{h-2}). \qquad (7.19) \end{aligned}$$

But $B_h = a_h B_{h-1} + \epsilon_h B_{h-2} = 2B_{h-1} - B_{h-2}$ by (7.17). Hence

$$B_{h-2} + B_h = 2B_{h-1}. \tag{7.20}$$

Then (7.19) and (7.20) give

$$B_{2h-1} = -B_h B_{h-2} + 2B_{h-1}^2,$$

which is the second equation of the PQ-test.

We now verify the third equation of each of the three tests. Recall equation (5.3):

$$A_{k-1}^2 - DB_{k-1}^2 = (-1)^k \epsilon_1 \cdots \epsilon_k. \tag{7.21}$$

Hence if $k = 2h$ and D is of Type I, then (7.21) and the symmetries (7.9) and (7.10) give

$$A_{k-1}^2 - DB_{k-1}^2 = 1,$$

which corresponds to the third equation of the P-test.

Assume $k = 2h+1$. If $k = 1$, then (a) $D = t^2+1, t \geq 1$ or (b) $D = t^2-1, t > 1$. In both cases $A_0 = t, B_0 = 1$, while in case (a), $\epsilon_1 = 1$ and case (b), $\epsilon_1 = -1$ and we see that the third equation of the Q-test is satisfied.

If $k > 1$, equation (7.21) and the symmetries (7.7) and (7.8) give

$$A_{k-1}^2 - DB_{k-1}^2 = -\epsilon_{h+1},$$

which again is the third equation of the Q-test.

Finally if $k = 2h$ and the continued fraction is of Type II, then (7.21) and $\epsilon_h = -1, \epsilon_{h+1} = 1$ and symmetries (7.9) and (7.10) otherwise, give

$$A_{k-1}^2 - DB_{k-1}^2 = -1,$$

which corresponds to the third equation of the PQ-test.

Remark. If $\xi_0 = (1+\sqrt{D})/2, D \equiv 1 \pmod 4$, we also have P, Q and PQ tests, with the Pell equations replaced, as follows: If k is the period-length, then

$$\begin{aligned} \text{P} &: A_{k-1}^2 - A_{k-1}B_{k-1} - \tfrac{(D-1)}{4}B_{k-1}^2 = 1; \\ \text{Q} &: A_{k-1}^2 - A_{k-1}B_{k-1} - \tfrac{(D-1)}{4}B_{k-1}^2 = -\epsilon_{h+1}, k = 2h+1; \\ \text{PQ} &: A_{k-1}^2 - A_{k-1}B_{k-1} - \tfrac{(D-1)}{4}B_{k-1}^2 = -1. \end{aligned}$$

The above proofs go through; except if $k = 1$, then (a) $D = t^2+4, t \geq 3$, t odd or (b) $D = t^2-4, t \geq 3$, t odd. In both cases $A_0 = (t+1)/2, B_0 = 1$, while in case (a), $\epsilon_1 = 1$ and case (b), $\epsilon_1 = -1$.

Remark. The reduced period π of Williams and Buhr ([13, p. 373]) can be shown to be equal to k, the NSCF period-length of $\sqrt{D}$. From [13, p. 374], the following hold:

(a) Conditions 1 and 2 satisfy the P-test for $\sqrt{D}$;
(b) Conditions 3, 4 and 5 satisfy the Q-test for $\sqrt{D}$;
(c) Condition 6 satisfies the PQ-test for $\sqrt{D}$.

8. Numerical results

In Table 1, we give the frequency of occurrence of each of three criteria for the NSCF expansion of $\sqrt{D}$ for non-square $D \leq M$.

Table 1. Frequency of P, Q and PQ criteria for $\sqrt{D}, D \leq M$.

M	P-test	Q-test	PQ-test	Total
100	60	25	5	90
1000	762	165	42	969
10000	8252	1266	382	9900
100000	85856	10465	3363	99684
1000000	878243	90533	30224	999000
10000000	8915623	805295	275920	9996838

TABLE 2. RCF and NSCF continued fraction expansions of $\sqrt{97}$.

j	i	ξ_i	ξ'_j	ϵ_i	a_i	a'_j	A_i/B_i	A'_j/B'_j
0	0	$\frac{0+\sqrt{97}}{1}$	$\frac{0+\sqrt{97}}{1}$	1	10	9	10/1	9/1
1			$\frac{9+\sqrt{97}}{16}$			1		10/1
2	1	$\frac{10+\sqrt{97}}{3}$	$\frac{7+\sqrt{97}}{3}$	-1	7	5	69/7	59/6
3			$\frac{8+\sqrt{97}}{11}$			1		69/7
4	2	$\frac{11+\sqrt{97}}{8}$	$\frac{3+\sqrt{97}}{8}$	-1	3	1	197/20	128/13
5			$\frac{5+\sqrt{97}}{9}$			1		197/20
6	3	$\frac{13+\sqrt{97}}{9}$	$\frac{4+\sqrt{97}}{9}$	-1	2	1	325/33	325/33
7	4	$\frac{5+\sqrt{97}}{8}$	$\frac{5+\sqrt{97}}{8}$	1	2	1	847/86	522/53
8			$\frac{3+\sqrt{97}}{11}$			1		847/86
9	5	$\frac{11+\sqrt{97}}{3}$	$\frac{8+\sqrt{97}}{3}$	-1	7	5	5604/569	4757/483
10			$\frac{7+\sqrt{97}}{16}$			1		5604/569
11	6	$\frac{10+\sqrt{97}}{1}$	$\frac{9+\sqrt{97}}{1}$	-1	20	18	111233/11294	105629/10725
12			$\frac{9+\sqrt{97}}{16}$			1		111233/11294
13	7	$\frac{10+\sqrt{97}}{3}$	$\frac{7+\sqrt{97}}{3}$	-1	7	5	773027/78489	661794/67195

TABLE 3. Comparison of NSCF and RCF periods for $\sqrt{D}$.

n	$\Pi(n)$	$P(n)$	$\Pi(n)/P(n)$
1000000	152198657	219245100	.6941941
2000000	417839927	601858071	.6942499
3000000	755029499	1087529823	.6942609
4000000	1149044240	1655081352	.6942524
5000000	1592110649	2293328944	.6942356
6000000	2078609220	2994112273	.6942322
7000000	2604125007	3751067951	.6942356
8000000	3165696279	4559939520	.6942408
9000000	3760639205	5416886128	.6942437
10000000	4387213325	6319390242	.6942463

In Table 2, $D = 97$ and the NSCF expansion of $\sqrt{97}$ is of type II, with period length 6. There are 5 negative ϵ_i's in the period range $1 \le i \le 6$ and the period length of the RCF expansion of $\sqrt{97}$ is 11.

In Table 3, we compare $\pi(D)$ and $p(D)$, the respective periods of the NSCF and RCF expansions of $\sqrt{D}$, where D is not a perfect square. We let

$$\Pi(n) = \sum_{D \le n} \pi(D), \quad P(n) = \sum_{D \le n} p(D).$$

Then it appears that $\Pi(n)/P(n) \to \tau = \log_2\left(\frac{1+\sqrt{5}}{2}\right) = .6942419\cdots$

The limiting behaviour in Table 3 was also observed for the nearest integer continued fraction by Williams and Buhr ([13, p. 377]) and Riesel ([10, p. 260]). In fact one can show that the period-lengths of the nearest square and nearest integer continued fraction expansions of a quadratic irrationality are equal (see [6]). Also if X/Y is the smallest solution of Pell's equation $x^2 - Dy^2 = \pm 1$, then X/Y has regular continued fraction expansion

$$X/Y = a_0 + \frac{1}{\lceil a_1} + \cdots + \frac{1}{\lceil a_{p(D)-1}} \tag{8.1}$$

and nearest integer continued fraction expansion

$$X/Y = b_0 + \frac{\epsilon_1}{\lceil b_1} + \cdots + \frac{\epsilon_k}{\lceil b_{\pi(D)-1}}. \tag{8.2}$$

By theorems of Heilbronn and Rieger (see [9, p. 159]), for D with a long RCF period, we expect the ratio $\pi(D)/p(D)$ of the lengths of these finite continued fractions to approximate τ. For example, with $D = 26437680473689$ (an example of Daniel Shanks [11] with a long RCF period) we have $p(D) = 18331889$, $\pi(D) = 12726394$, $\pi(D)/p(D) = .6942216\cdots$.

9. Computational tests

We conclude with a comparison of the computational performance of continued fraction algorithms and consider the question of which of the three CF algorithms (RCF, NICF, NSCF) is the more computationally efficient for solving the Pell equation for any given value of D. All tests were performed on a Sun Sparcv9 processor (750MHz). The programs were written in C and used the GMP (Version 4.2.4) multiple precision arithmetic library for convergent calculations.

Two versions of each algorithm were tested, a "standard" version and a "quotient-optimised" version. In both versions, we employ some fairly obvious optimisations such as developing only one convergent sequence B_n, then solving directly for the corresponding A_n once only at the conclusion of the main loop. This typically halves the amount of processing that would be required if we had developed both sequences.

In the "standard" programs, the calculation of each $B_n = a_n B_{n-1} \pm B_{n-2}$ is performed in two steps, a multiplication giving $a_n B_{n-1}$ followed by the addition/subtraction of B_{n-2}. The quotient-optimised versions use two distinct time-saving optimisations to this process. The first improvement is to introduce special handling of partial quotient values 1, 2 and 4. These can benefit from special handling, and also occur with sufficient frequency to make this well worthwhile.

In the RCF, for example, a partial quotient value of 1 occurs with average frequency 41.5%. Computing the new convergent thus requires only the addition of the previous two values, avoiding an unnecessary multiplication. In all three algorithms, partial quotient values of 2 and 4 can benefit from using the special GMP function for multiplication by powers of 2. This function uses shift instructions to perform the operation, and these are usually faster than normal multiplication.

For all other quotient values, improvement over the standard version is also obtained, by using a GMP function that gives a combined multiply-and-add (or subtract) operation, allowing the convergent calculation to be performed as a single step.

The first set of test results involve "short-period" tests. We processed all values of D in the range $[10^6(n-1), 10^6 n]$ for $n = 1$ to 6. Table 4 lists the results obtained using the standard convergent method. Times are given in seconds, and for NICF and NSCF, the times relative to RCF are also given.

We also ran a set of "long-period" tests. Here we processed specific values D_n of D with substantially long period lengths. The specific values and corresponding period lengths are listed in Table 5. Note that the period length ratios in each case are all very close to the expected average of .694.

Table 6 lists the solution times for each D_n in seconds, using the standard convergent method, with the ratios of times for NICF and NSCF relative to the corresponding RCF times.

With the standard method of convergent calculation, our main observations are these:

(a) there is no significant difference between NICF and NSCF;
(b) as period lengths increase, the relative performance of NSCF and NICF against RCF is increasingly close to the corresponding ratio of period lengths.

These results generally conform with expectations - as period lengths increase, the computational cost is increasingly dominated by the cost of calculating the convergents, with both NSCF and NICF performing exactly the same number of convergent calculation steps.

A different trend becomes evident, however, when the same tests are performed using the quotient-optimisation method. Tables 7 and 8 show the corresponding results using this method.

TABLE 4. Short-period times for $[10^6(n-1), 10^6 n]$ (standard method).

n	RCF	NICF	ratio	NSCF	ratio
1	81	64	.790	64	.790
2	147	118	.803	120	.816
3	200	160	.800	162	.810
4	248	196	.790	199	.802
5	291	230	.790	232	.797
6	334	258	.772	255	.763

TABLE 5. Long-period D_n examples.

n	D_n	RCF period-length	NSCF-NICF period-length
1	$10^{14}+3$	625024	433550
2	$10^{14}+7$	869844	604092
3	$10^{12}+24$	1005170	697848
4	$10^{12}+189$	2064689	1433367
5	$10^{12}+294$	2963566	2057350

TABLE 6. Long-period times for D_n (standard method).

n	RCF	NICF	ratio	NSCF	ratio
1	63	43	.683	43	.683
2	133	93	.699	93	.699
3	181	126	.696	126	.696
4	850	592	.696	589	.693
5	1797	1251	.696	1246	.693

TABLE 7. Short-period times for $[10^6(n-1), 10^6 n]$ (Quotient-optimised).

n	RCF	NICF	ratio	NSCF	ratio
1	56	54	.964	54	.964
2	102	101	.990	102	1.000
3	136	135	.993	135	.993
4	165	165	1.000	165	1.000
5	193	195	1.010	196	1.016
6	218	221	1.014	224	1.028

TABLE 8. Long-period times for D_n (Quotient-optimised).

n	RCF	NICF	ratio	NSCF	ratio
1	31	35	1.129	35	.964
2	65	72	1.108	73	1.123
3	90	100	1.111	100	1.111
4	398	468	1.176	467	1.173
5	880	986	1.120	987	1.122

All three CF algorithms benefit substantially from quotient optimisation, but it is RCF that benefits the most. At short period lengths it now performs just as well as NICF or NSCF, and as period lengths increase it becomes noticably faster. This can be explained by examining the average relative frequencies of quotient occurrences for the values in question.

Quotient values of 2 or 4 occur around 23% of the time for RCF, and 33% for NICF and NSCF. What tips the balance in favour of RCF is the 41.5% frequency of quotient value 1, which never occurs at all with NICF or NSCF. The optimisation for this particular case is also the one that is most beneficial, as it avoids multiplication altogether.

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