MIDPOINT TWO- STEPS RULE FOR THE SQUARE ROOT METHOD

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ABSTRACT

We present a method "Midpoint-Two-Steps rule" for the square root functional iteration for enclosing zeros of a polynomial. The method combines classical square root method in its formulation a variant of the approach adopted by (Wang and WU,1985) where a Gauss-Siedel updating formula was used to accelerate the well known Meahly – Aberth third order method for finding zeros of a polynomial in interval arithmetic. Our method has the capability of converging faster than the classical square root and Meahly-Aberth third order methods. This was possible since the predictor and corrector iterations which the algorithm entails do not jump across paths of orientation. The convergence of the midpoints and radii of the including disks which the presented method entails for the sequence of solution are coupled via the inclusion isotonicity property of circular interval arithmetic.

Interestingly, it was proved that the midpoint-two steps rule for the square root method converges if and only if the second order derivative of the polynomial P(z) is inverse forcing. Theoretical numerical example has been demonstrated with constructed algorithm with high substantial of probability 1.

KEY WORDS: Square root iteration, midpoint two steps Method, Meahly-Aberth-Third Order Method, polynomial zeros, Circular Interval Arithmetic.

1. INTRODUCTION

The paper develops algorithm for the numerical approximation of zeros of polynomial. The proposed method combines classical square root functional iteration in such a way that, the obtained method may be viewed as a class of q-steps method in the sense of (Wang and WU, 1985). Such composite procedures provide tight inclusion intervals separating the sought zeros. We emphasize that the task of computing simultaneously zeros of a polynomial whose initial starting roots are expressed in the form of intervals is NP-hard even for n=2. We then define the concept of an interval in Mathematics as a natural extension of that of a scalar. A scalar value is a discreet point but an interval is a continuum defined by two scalar end values. We naturally think of an interval type as being derived from a scalar type, in which case we refer to the scalar type as the base type, (Uwamusi,1998). For example, if a and b are base type that define the scalar end values of an interval, then that interval is written [a, b]. Like any other numerical mathematics, the interval type has a rich set of arithmetic operators (Moore, 1966) associated with it including binary operators for the basic operations of addition, subtraction, multiplication and division.

Let [a, b] and [c, d] be the two operands of a binary operator, then following (Moore,1966) the four basic arithmetic operators are defined by

Addition : [a,b]+[c,d] = [a+c,b+d]

Subtraction : [a,b] - [c,d] = [a-d,b-c]

Multiplication: $[a,b] \times [c,d] = [\min, Max]$

where

min = minimum $(a \times c, a \times d, b \times c, b \times b)$,

max = maximum $(a \times c, a \times d, b \times c, b \times b)$

division $[a,b] \div [c.d]$

$$=[a,b] \times \left[\frac{1}{d}, \frac{1}{c}\right]$$

The unary versions of the addition and subtraction operators follow by noting that +[a,b] = [0,0] + [a,b] and -[a,b] = [0,0] + [-a,-b], where 0 denotes the additive identity value for the base

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type. It should be noted that for certain base types, for example, points on the real axis, there is some sense of an interval lower bound and a corresponding upper bound. We point out here that such properties do not necessarily hold for all base types (for example, points in the complex plane). Hence in the following, we do not rely in the existence of comparison operators, such as a
b or in the interval [a,b],b must be greater than a in some sense, (Uwamusi,1998). Since the interval type supports a full set of arithmetic operators, values of this type may be combined in arithmetic expression, in the same way as values of other numeric types, such as base types of the interval itself, (Uwamusi,1998). There exist three types of interval arithmetic – the complex, the circular and rectangular arithmetic. We shall be interested in the circular arithmetic due to (Gargantini and Henrici ,1972). To describe this, we review:

Definition (Gargantini and Henrici, 1972): A circular region denotes a closed point set in the extended complex plane whose projection on the Rieman sphere is bounded by a circle. Depending whether the point infinity is an exterior point, a boundary point, or an interior point, a circular region thus is either a closed disk, a closed hall-plane, or the complement of an open disk.

Let $Z = \{z : |z - c| \le r\}$ where Z denotes a disk, c is the midpoint of Z and r is the radius. Then there follows the basic properties of circular interval arithmetic we shall need in the paper:

$$\{c_1, r_1\} \pm \{c_2, r_2\} = \{c_1 + c_2, r_1 + r_2\}$$
(1.1)

$$\{c_1, r_1\}.\{c_2, r_2\} = \{c_1 c_2, |c_1| r_2 + |c_2| r_1 + r_1 r_2$$
(1.2)

$$\frac{1}{\{c-r\}} = \frac{\left\{\bar{c}-r\right\}}{\left|c\right|^2 - r^2}, \quad (\left|c\right| > r)$$
(1.3)

$$\{c,r\}^{n} = \left\{c^{n}, \sum_{j=1}^{n} {n \choose j} |c|^{n-j} r^{j}\right\}$$

= $\left\{c^{n}, (|c|+r)^{n} - |c|^{n}\right\}$ (1.4)

The k-th root of a disk is

$$\{c,r\}^{\frac{1}{k}} = \left[\frac{1}{c^{\frac{1}{k}}}, \frac{r}{|c|^{\frac{1}{k}} + (|c| - r)^{\frac{1}{k}}}\right], (k \in N, |c| > r).$$
(1.5)

Let us note that

$$rad \left(\frac{1}{Z^{\frac{1}{k}}}\right) \leq rad \left(\frac{1}{Z}\right)^{\frac{1}{k}}, \left(0 \notin Z\right),$$
(1.6)

where rad (Z) denotes the radius of the disk Z. Inclusion isotonicity of circular interval arithmetic is defined by the expression

$$\{c_1, r_1\} \subseteq \{c_2, r_2\} \Longrightarrow |c_1 - c_2| \le r_1 - r_2$$
 (1.7)

In this paper we will adopt the disk inversion due to (Carstensen and Petkovic, 1994) assuming that $0 \notin Z$ and |c| > r in the form

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$$Z^{-1} = \{c, r\} = \left[\frac{1}{c\left(1 - \frac{r^2}{|c|^2}\right)}, \frac{r}{|c|^2 - r^2}\right]$$
(1.8)

$$Z^{I_1} = \{c, r\}^{I_1} = \left\{\frac{1}{c}, \frac{r}{|c|(|c|-r)|}\right\},$$
(1.9)

$$Z^{I_2} = \{c, r\}^{I_2} = \left\{ \frac{1}{c}, \frac{2r}{|c|^2 - r^2} \right\}$$
(1.10)

Thus $Z^{-1} \subseteq Z^{I_1} \subseteq Z^{I_2}$ and the estimates

$$|mid(Inv_i(Z))| \le \frac{|c|}{|c|^2 - r^2}$$
 (1.11)

$$rad (InV_i(Z)) \le \frac{2r}{|c|^2 - r^2}$$
(1.12)

are valid for any disk inversion, where $InV_i(Z)$ denotes any of the three inversions, Z^{-1} , Z^{I_1} and Z^{I_2} . Note that $mid (Z^{-1}) \neq mid(Z)^{-1}$ in general.

It follows that the disk to be chosen in the evaluation of $Z^{\frac{1}{2}}$ requires the calculation of $P^{1}(z_{i}^{(o)})/P(z_{i}^{(o)})$.

Our interest in this work is also the specification of a polynomial and the corresponding roots of that polynomial. Thus a polynomial is a combination of powers of some z. We choose to use $a_{n-1},...,a_0$ to denote coefficients in this linear combination and write

$$P_n(z) = a_n z^n + a_{n-1} z^{n-1} + \dots + a_1 z + a_0$$

Because we are interested in the roots of $P_n(z)$ (i.e. the values of z for which $P_n(z)=0$), the choice of a_n , the leading coefficient of $P_n(z)$ as 1 can be made without loss of generality. Such polynomial is called a monic polynomial, which has several uses in Sciences and Engineering, for example in the building block of companion matrices e.g.; (Carstensen 1991).

We also need to specify in advance the type of polynomial coefficients and also the type of the variable z.

It is clear that it must be necessary to perform multiplication between values of these types if operations such as polynomial evaluation and the evaluation of the derivatives are to be possible. It can be expected that one of these is a generalization of the other, and hence it is possible to regard a polynomial as involving a single types only. Even if the coefficients of a polynomial are real, the roots of that polynomial may be complex and hence it is convenient to regard all roots as being complex, with the real roots having imaginary part. In this paper we are interested in locating the roots of a polynomial with real coefficients only. The roots themselves are to be computed using circular arithmetic a variant of (Moore, 1966), interval arithmetic operation earlier mentioned.

The remaining parts in the paper are arranged as follows: In section 2 we described the method and the methodology adopted. In particular we proved that convergence of Midpoint –Two steps rule holds if and only if the second order derivative of the polynomial, P(z) is inverse forcing. In section 3 we demonstrated the method with a theoretical example while the paper is concluded based on the findings from the method in comparison with results from known method.

2. METHODOLOGY: The Method.

Let P denote a polynomial of degree $n \ge 3$ defined as

$$P_{n}(z) = \sum_{j=1}^{n} a_{j} z^{j} = \prod_{j=1}^{n} (z_{i} - \xi_{j}), \ (a_{j} \in \mathcal{I}),$$

with leading coefficient unity where $\xi_1, \xi_2, ..., \xi_n$ represent real or complex zeros and the polynomial p is exact, is in solution space of Laguerre hyper plane (Gargantini and Henrici ,1972), (Petkovic and Stefanovic ,1984) in the sense that $z_1 + z_2 + ... + z_m = a_{n-1}$.

Following closely the ideas in (Gargantini and Henrici, 1972), we introduce the function number of zeros is exact that can be estimated by Lagouanelle's limiting formula in the sense of (Farmer and Loizou ,1977), such that the number of zeros $(z_1, z_2, ..., z_n)(m < n)$ of the

$$F_{r}(z) = \frac{(-1)^{r-1}}{(r-1)!} \frac{d^{r}}{dz^{r}} \log_{e} p(z), (r \ge 1) , \qquad (2.1)$$

to designate the logarithmic derivative of p(z) for the case of simple zeros. The case of multiple zeros can also be found in (Petkovic, 989). We note in passing that the procedure for deciding if a polynomial has real or complex roots has been discussed in the excellent book by (Ostrowski,1970), and for this, we omit.

It is easily verified from (2.1) that

$$F_r(z) = \sum_{j=1}^n \frac{1}{(z - \xi_j)^r} \quad .$$
 (2.2)

If all zeros of the polynomial p except ξ_i are known, what can be said about the unknown zero? From the knowledge of separation axioms of Hausdorff topological space it is known that the unknown zero ξ_i is in the open set and is given by the relation (Gargantini and Henrici, 1972)

$$Z_{i}^{(k+1)} = z_{i}^{(k)} - \frac{1}{\left[F_{r}\left(z_{i}^{(k)}\right) - \sum_{\substack{j=1\\j\neq i}}^{n} \left(\frac{1}{z_{i}^{(k)} - Z_{i}^{(k)}}\right)^{r}\right]_{+}^{\frac{1}{2}}$$
(2.3)

 $(i = 1, 2, ..., n, k = 0, 1, ..., r \in N)$

Observe that the symbol + denotes the choice of only one disk among r disks that appear as the r^{th} root sets of the disk in the denominator (2.3), (Gargantini and Henrici ,1972), (Petkovic ,1989). Because $z_1^{(o)}$ does not belong to any of the disks $Z_i^{(o)}$, *then* $(z_1^{(o)} - Z_j^{(o)})$ does not contain the origin and its inverse is a disk. The inverse operation is exact but the square of $(Z_1^{(o)} - Z_j^{(o)})^{-1}$ is however in general too large a region to be a disk Gargantini and Henrici (1972).

Thus the criterion for the choice of a proper disk is analyzed in Petkovic (1989). It reads as follows:

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"Let
$$\left[F_2(Z_i^{(k)}) - \sum_{\substack{j=1\\j\neq i}}^n \left(\frac{1}{z_i^{(k)} - Z_i^{(k)}}\right)^2\right]^{1/2} = D_{1i}^{(k)} \cup D_{2i}^{(k)}$$
 and, $D_{1i}^{(k)}$ and $D_{2i}^{(k)}$ be found according to the square root

method in section 1. Therefore, of the two disks $D_{1i}^{(k)}$ and $D_{2i}^{(k)}$ one chooses the disk whose centre is able to $|p'(z_i^{(k)})| = 1 - |p| (z_i^{(k)})$

minimize
$$\left| \frac{p(z_i^{(k)})}{p(z_i^{(k)})} - mid D_{v,i}^{(k)} \right|, (v = 1,2).$$
"

-

Let us note that if we ignore the sum in iterative formula appearing in equation (2.3) we will be led to (Ostrowski, 1970)

formula
$$z_i^{(k+1)} = z_i^{(k)} - \frac{1}{\left(F_2(z_i^{(k)})\right)^{\frac{1}{2}}}$$
 with a cubic order of convergence, (Petkovic and Stefanovic, 1984).

Now for r=1 in method (2.3, we obtain the well known Meahly-Aberth third order method (Gargantini and Henrici, 1972) which is traced to Newton's method; in the form :

$$Z_{i}^{(k+1)} = z_{i}^{(k)} - \frac{1}{\frac{p'}{p} - \sum_{\substack{j=1\\j\neq i}}^{n} \frac{1}{z_{i}^{(k)} - Z_{j}^{(k)}}}.$$
(2.4)

We shall be interested when r=2 as in the case of simple zeros. Hence we write

$$Z_{i}^{(k+1)} = z_{i}^{(k)} - \frac{1}{\left[F_{2}(z_{i}^{(k)}) - \sum_{\substack{j=1\\j \neq i}}^{n} \frac{1}{(z_{i}^{(k)} - Z_{j}^{(k)})^{2}}\right]^{\frac{1}{2}}}$$
(2.5)

In what follows we introduce the Midpoint –Two steps method, a variant of the approach adopted by (Wang and WU ,1985), (see also the analysis given by (Petkovic ,1989) wherein they applied a Gauss-Siedel type update to Meahly-Aberth third order method.

Thus (2.5) can be rewritten in the form:

$$Z_{i}^{\left(k+\frac{\lambda+1}{q}\right)} = z_{i}^{\left(k+\frac{\lambda}{q}\right)} - \frac{1}{\left[F_{2}\left(z_{i}^{\left(k+\frac{\lambda}{q}\right)}\right) - \frac{1}{\sum_{\substack{j=1\\j\neq i}}^{n} \left(z_{i}^{\left(k+\frac{\lambda}{q}\right)} - Z_{j}^{\left(k+\frac{\lambda+1}{q}\right)}\right)^{2}\right]^{\frac{1}{2}}}$$
(2.6)

 $(k = 0, 1, ..., \lambda = 0, 1, ..., q - 1, q = 2, 3, ..., t)$

q is an integer and the most popular choice of q is 2 due to high computational complexity of computing higher derivatives of F. Experimental results showed that higher values of q really do not contribute significantly to the convergence speed of the algorithm, (Uwamusi, 2004).

Method (2.4) can be modified by adding Newton's correction $N_j (= p / p')$ to the disk in the form $Z_j = Z_j - N_j$ Hence method (2.4) becomes

$$Z_{i}^{(k+1)} = z_{i}^{(k)} - \frac{1}{N_{i}^{-1} - \sum_{\substack{j=1\\j \neq i}}^{n} \frac{1}{z_{i}^{(k)} - Z_{j}^{(k)} + N_{j}}}$$
(2.7)
(k-0,1,..).

It is well known (Carstensen and Petkovic, 1994) that the disk in method (2.7) does not contain the origin and its inversion exists since $z_i^{(o)}$ and $Z_j^{(o)}$ belong respectively to disjoint open sets. For this, we are able to prove:

Theorem: 2.1

The square root method converges if and only if the term $F_2(z_i^{(k)})$ is inverse forcing. This means that $F_2(z_i^{(k)})^{-1} \to 0$, as $k \to \infty$ both the midpoint of the including disk (i.e. mid (Z_j) and rad (Z_i) are coupled as the sequence $(z_i)_{i=1}^{\infty}$ approaches the desired zeros of polynomial, P.

Proof:

The convergence follows the fact that $F_2(z_i^{(k)})$ becomes very large compared to Laguerell's correction

$$L_i^{(k)} = \sum_{\substack{j=1\\j\neq i}} \left(\frac{1}{z_i^{(k)} - Z_j^{(k)}}\right)^2$$

as the sequence of iterate approaches infinity.

By setting $G_i^{(k)} = \left(F_2(z_i^{(k)}) - L_i^{(k)}\right)$, then we compute $\sqrt{G_i^{(k)}}$ to be

$$\sqrt{G_{i}^{(k)}} = \left\{ \pm \sqrt{midG_{i}^{(k)}} , \frac{rad \ G_{i}^{(k)}}{\sqrt{\left|midG_{i}^{(k)}\right| + \sqrt{\left|mid \ G_{i}^{(k)}\right| - radG_{i}^{(k)}}\right)}} \right\}$$

In the limit, the correction term of the square root method tends to $\left(\sqrt{\left|midG_{i}^{(k)}\right|}\right)^{-1}$ while the radius $\frac{rad \ G_{i}^{(k)}}{\sqrt{\left(midG_{i}^{(k)}\right) + \sqrt{\sqrt{\left(G_{i}^{(k)}\right| - radG_{i}^{(k)}\right)}}} \rightarrow 0 \ as \ k \rightarrow \infty$. This implies that the radius becomes vanishingly small in

magnitude. Thus the radius and midpoint of Z_i are coupled as $k \to \infty$.

The order of convergence of method (2.6) is equal to 3+ $\delta_n(z)$ and is the unique positive zero of $\delta^n - \delta - 3 = 0$, and it is $2 + \delta_n(z) = \delta^n - \delta - 2 = 0$ in the case of (2.5). This was obtained from the spectral radius of the matrix

$$A = \begin{bmatrix} r+1 & 1 & \dots & 0 \\ r+1 & 1 & \dots & 0 \\ & & \dots & 0 \\ r+1 & 1 & 0 \dots & r+1 \end{bmatrix}$$

by the well known power method $y^{(m+1)} = Ay^{(m)}$. (2.8)

Starting with the vector $y^{(0)} = (1,1,...,1)^T$. The spectral radius of A is given by $\rho((A) = r + 1 + \delta_n(r))$, is also the lower bound of the R-order of convergence of method (2.5).

The speed up in the computation of (2.8) may be enhanced by the aid of Aiken Δ^2 method (see,(Burden and Fairs ,1993) for details). We remark that the efficiency of method (2.5) is obtained when r=2 as higher values of r>2 may call for higher computational efforts in evaluating higher derivatives of p and we know that computing zeros of polynomials with interval methods is computationally NP- complete, (Neumaier, 1990).

Note that in the case of complex roots, we need the calculation of $|c| = |p + iq| = (p^2 + q^2)^{\frac{1}{2}}$

since |c| > r, then may require us to rewrite $\frac{r}{|c|(|c|-r)|}$ as

 $\frac{r}{|c|(c)-r|} = \frac{r(1+r/|c|)}{|c|^2-r^2} < \frac{2r}{|c|^2-r^2}.$ As a result of the above, it follows that rad $(c,r)^{I_2} = 2rad(c,r)^{-1}.$ This increase

of the radius of the inverse disks causes certain problems if the initial disks are not small enough. Following (Carstensen and Petkovic ,1994) we remember that the approximation $p < \frac{1}{2}(1 + p^2)$, where 0 will

result in the following expression

$$\frac{r}{|c|(|c|-r)|} < \frac{r\left(\left(1 + \frac{1}{2}\left(1 + r^2/|c|^2\right)\right)\right)}{|c|^2 - r^2} = \frac{r\left(\frac{3}{2} + \frac{1}{2}r^2/|c|^2\right)}{|c|^2 - r^2} < \frac{2r}{|c|^2 - r^2}$$

In this case the disk to be inverted has the form.

$$\{z,r\}^{i^2} = \left(\frac{1}{c}, \frac{r\left(\frac{3}{2} + \frac{1}{2}r^2 / |c|^2\right)}{|c|^2 - r^2}\right).$$
(2.9)

From experimental survey it is found out that the application of disk inversion using method (2.9) is likely to fail,(Uwamusi, 2008) if the initial disk is not large enough in the sense that divergence may occur, when the diameter of the disk $z_i^{(k)}$ is very small which also formed part of our investigation in the paper.

3. THEORETICAL EXAMPLE

Consider the polynomial problem taken from (Gargantini and Henrici, 1972) given by

$$P(z) = z^3 - 2z^2 - z + 2 \, .$$

The initial including intervals are

 $Z_i^{(0)} = [2.2, 0.3], Z_2^{(0)} = [0.9, 0.2], Z_3^{(0)} = [-0.9, 0.3]$

The following results have been obtained from the theoretical problem.

Table 1. Square root method (2.5)

$$Z_{1}^{(1)} = \{2.00025768, -0.000781835\}$$

$$Z_{2}^{(1)} = \{0.99994181, 0.000119753\}$$

$$Z_{3}^{(1)} = \{-1.000013289, 0.00047874\}$$

$$Z_{1}^{(2)} = \{2.000000001, 2.323958276 \times 10^{-15}\}$$

$$Z_{2}^{(2)} = \{0.999998817, -1.57411123 \times 10^{-16}\}$$

$$Z_{3}^{2} = \{-1.000000000, 5.286992099 \times 10^{-15}\}$$

Table 2 Midpoint-Two step rule for square root method (2.6)

 $Z_{1}^{\frac{1}{2}} = \{2.00025768, -0.000781835\}$ $Z_{2}^{\frac{1}{2}} = \{1.000024602, -0.000050497\}$ $Z_{3}^{\frac{1}{2}} = \{-0.99999985, -0.000000039\}$ $Z_{1}^{(1)} = \{2.000000001, 8.631845019 \times 10^{-16}\}$ $Z_{2}^{(1)} = \{1.00000000, 0\}$ $Z_{3}^{(1)} = \{-1.000014985, 0\}$

Table 3 Meahly-Aberth Third Order Method (2.7)

 $Z_{1}^{(1)} = \{2.003799143, -0.005158613\}$ $Z_{2}^{(1)} = \{1.000366236, -0.003357169\}$ $Z_{3}^{(1)} = \{-0.988815126, -0.003357169\}$ $Z_{1}^{(2)} = \{1.999999999, 0.000000049\}$ $Z_{2}^{(2)} = \{0.999999866, 7.17006282 \times 10^{-10}\}$ $Z_{3}^{2} = \{-1.000084343, -0.00000181\}$

4. CONCLUSION

From tables 1-3, it can be observed that the results obtained approximate very closely the true zeros of p with high substantial of probability 1.That means the presented method we proposed is sure to converge on any zeros of polynomial P (z) if the initial including disks are well separated and non of the denominators appearing in the correction formulas contain the origin. We have illustrated the immunity of these interval methods to a theoretical problem which illustrates that the presented methods can also be of practical use other than the theoretical example given and that the dimension of the polynomial problem is not an intrinsic limitation. It could be observed that from the experimental example, both the square root method (2.5) and the midpoint- two-steps rule for the square root method (2.6) performed substantially better than modified Newton's method (2.7). However, they require higher computational efforts than modified Newton's method. The square root method is greatly bedeviled by the choice of

which of the roots to choose in $\sqrt{G_1^{(k)}}$. Let us note that the task of computing the zeros of the given polynomial with initial including intervals by any known interval methods is NP-hard even for n=2. We attempted to verify the validation of including zeros of the given problem using disk inversion given in equation (2.9). Surprisingly enough, it corroborated what (Carstesen and Petkovic,1994) had opined earlier on that the initial disks must be well separated in order to avoid a pitfall. Finally, the q-steps method for square root functional iteration was found to have more appeals than the classical square root method. The only opportunity cost one has to pay is the computational complexity this method entails. This is more so since computing in interval arithmetic with self validating methods is known to be NP-hard in general.

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