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GENERALIZATIONS OF NEWTON'S METHOD

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Abstract

We give a survey of the complex dynamics of various generalizations of Newton's method for finding a complex root of a polynomial of a single variable.

1. ITERATION METHODS

The best known iteration method for finding a real or complex root of a function $g(z)$ is Newton's method. It consists of iterating the function

$$N(z) = z - \frac{g(z)}{g'(z)}$$

by starting with some initial approximation z_0 and defining the $(n+1)$ approximation by $z_{n+1} = N(z_n)$. If the function $g(z)$ is a polynomial (or a rational function), then the iteration function N will be a rational map of the form

$$N(z) = \frac{p(z)}{q(z)}$$

where $p(z)$ and $q(z)$ are polynomials with real or complex coefficients.

There are various important factors involved in choosing an iteration method to approximate the roots of a function. These include:

- *The Initial Value Problem.* For what initial values will the method converge? Will it converge to a root, and if so, which root?
- *The Rate of Convergence.* Will the convergence be quadratic or better near a root?
- *The Complexity of the Calculation.* Do first or higher derivatives have to be calculated?

We show how complex dynamics can shed light on some of these problems when using a Newton-type iteration for finding the real or complex roots of a polynomial in a single variable. We can illustrate the basins of attraction of the roots and the set of initial points for which the method will not converge. We can also determine some information about the order of convergence at a given root; in particular whether it is quadratic or not.

2. COMPLEX DYNAMICS OF ITERATION METHODS

It is useful to think of the iteration function N as being defined on the whole Riemann sphere, i.e. the complex numbers with the point at infinity adjoined. The global study of Newton's and other such methods can now be analyzed using the theory of the complex dynamics of rational maps on the Riemann sphere, that was started by G. Julia and P. Fatou in the 1920s.[1–6]

The *orbit* of a point z_0 is the set of iterates

$$\{z_0, z_1, z_2, z_3, \ldots\} = \{z_0, N(z_0), N(N(z_0)), \ldots\}.$$

The point z is a *fixed point* of N if $N(z) = z$. For the standard Newton's method applied to a polynomial g, each root of g will be a fixed point of N, and these will be the only finite fixed points. If g is not of degree 1, then ∞ will also be a fixed point of N.

The point z is a *periodic point* if $N^p(z) = z$, for some positive integer p. The least such integer p is called the *period* and the orbit of z is then a p-cycle. Note that a point of period 1 is a fixed point and a point of period p is a fixed point of the composite map N^p. A point z is *eventually periodic* if $N^k(z) = N^{k+p}(z)$ for positive integers k and p.

In Newton's method, we would like our initial point z_0 to converge to a fixed point that is a root. That certainly happens most of the time, but other things can happen. The orbit of z_0 could converge to a p-cycle, or it could wander chaotically about the Riemann sphere.

If z is a periodic point of period p, then the derivative $\lambda = (N^p)'(z)$ is called the *eigenvalue* of the periodic point z. It follows from the chain rule that λ is the product of the derivatives of N at each point on the orbit of z. Hence λ is an invariant of the orbit. A periodic orbit is called

attracting if	$\lvert\lambda\rvert < 1$,
super-attracting if	$\lambda = 0$,
repelling if	$\lvert\lambda\rvert > 1$, and
neutral if	$\lvert\lambda\rvert = 1$.

Using the Taylor's series for N, it can be shown that N will be linearly convergent at an attracting fixed point and at least quadratically convergent at a super-attracting fixed point. Recall that the sequence $\{z_n\}$ *converges linearly* to w if, for sufficiently large n, $|z_{n+1} - w| < c|z_n - w|$, where $0 < c < 1$, and it *converges quadratically* if, for sufficiently large n, $|z_{n+1} - w| < c|z_n - w|^2$, for some constant c.

If we are interested in the dynamics of N on the Riemann sphere, we can always conjugate N by an invertible linear fractional (Möbius) transformation T, and the dynamics of the iterates of N will be the same as the iterates of $T \circ N \circ T^{-1}$. On the Riemann sphere, the point at infinity is like any other point. In order to determine whether infinity is a fixed point of N and to find its eigenvalue there, we can conjugate N by the transformation $z \mapsto 1/z$ that interchanges 0 and ∞. Therefore the behavior of $N(z)$ at ∞ is the same as the behavior of $1/N(1/z)$ at 0.

The *basin of attraction* of a fixed point w of the map N is the set

$$\left\{ z \,\middle|\, \lim_{n\to\infty} N^n(z) = w \right\}$$

of all points that map to w under the iterates of N. This may have infinitely many components, and the *immediate basin of attraction* is the connected component containing the fixed point w.

The rational map N divides the Riemann sphere into two invariant sets, the *Julia set*, J_N, and its complement. The Julia set consists of points in which the dynamics of the iterations of N is complicated. Points in the complement of the Julia set will normally converge to a fixed point (that could be infinity), or to an attractive cycle. This complement could also contain a Siegel disk or Hermann ring in which the iterations are locally like an irrational rotation of a disk or an annulus.[5] The following properties of the Julia set are proven in the theory of the complex dynamics of a rational map.[1,3–5]

1. J_N is the closure of the repelling periodic points.
2. J_N is non-empty.
3. J_N is completely invariant under N; i.e. $N(J_N) = J_N = N^{-1}(J_N)$.
4. J_N is the boundary of the basin of attraction of each fixed point or attractive cycle.
5. If $w \in J_N$, then the closure of $\{z|N^n(z) = w$ for some non-negative integer $n\}$, the backward iterates of w, is the whole of J_N.

Property 4 guarantees that, if there are more than two roots, J_N will be a fractal set. Property 1 guarantees that the Julia set is an unstable set. Iterates of points close to the Julia set will move away from that set. Hence Newton's method is very sensitive to initial conditions when the initial point is near the Julia set. Nearby points could converge to different roots or might not converge at all. Ideally, if you start with a point actually on the Julia set, Property 3 implies that the iterates will also be on the Julia set. However in practice, because the Julia set is unstable, the iterates will most likely be thrown off the set because of rounding errors.

Does Newton's method converge to a root for practically every initial point? Unfortunately, the answer is no. The orbit could converge to an attractive cycle, rather than to a root.[7] In some of the generalizations of Newton's method that we shall consider, there may also be fixed points of the method that are not roots of the polynomial g; these are called *extraneous fixed points* and they may be attracting or repelling. McMullen[8] has shown that there is no single iterative rational root-finding algorithm that will work for almost all complex polynomials of degree larger than three. However, the roots of a polynomial of degree four or five, but not higher, can be computed using a tower of algorithms.[9]

The following theorem can be used to determine all the attractive cycles of N. A *critical point* of N is where the derivative vanishes; this is where N is not locally one-to-one.

Theorem.[1] *The immediate basin of an attractive fixed point or cycle of N contains the image of at least one critical point of N.*

If the maximal degree of the polynomials in the numerator and denominator of a rational function is d, then the function will have at most $2d-2$ critical points and hence at most $2d-2$ attractive cycles.

3. NEWTON'S METHOD

The standard *Newton's Method* is also called the *Newton-Raphson method.* Any root of the poly-

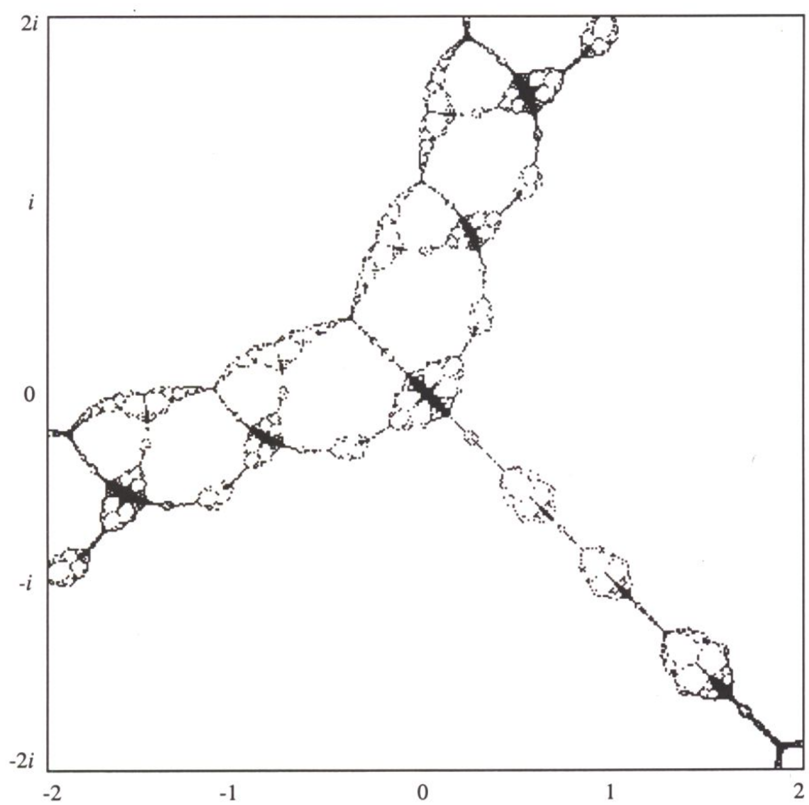

Fig. 1 The Julia set of Newton's method applied to $g(z) = (z-1)(z+i)(z+1-i)$.

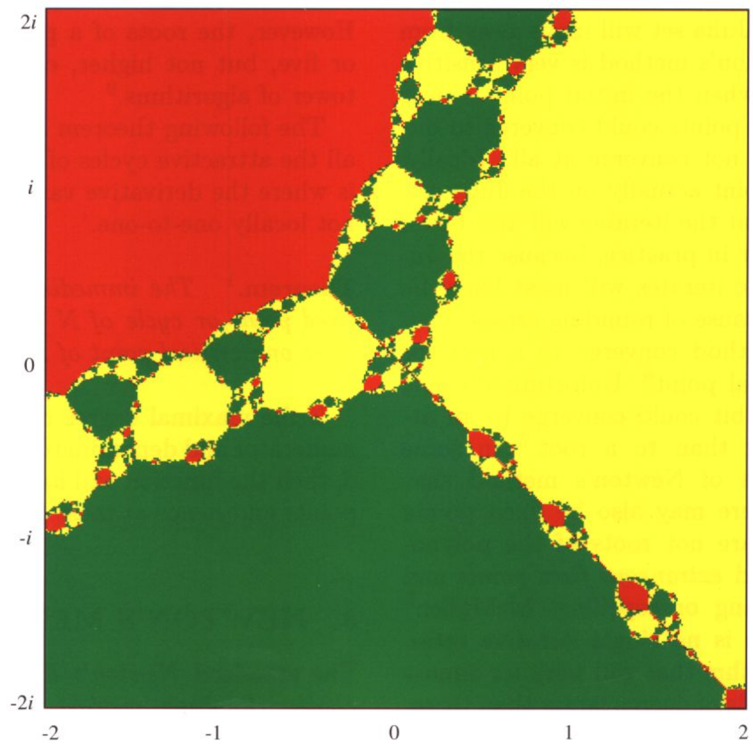

Fig. 2 Basins of attraction of Newton's method applied to $g(z) = (z-1)(z+i)(z+1-i)$.

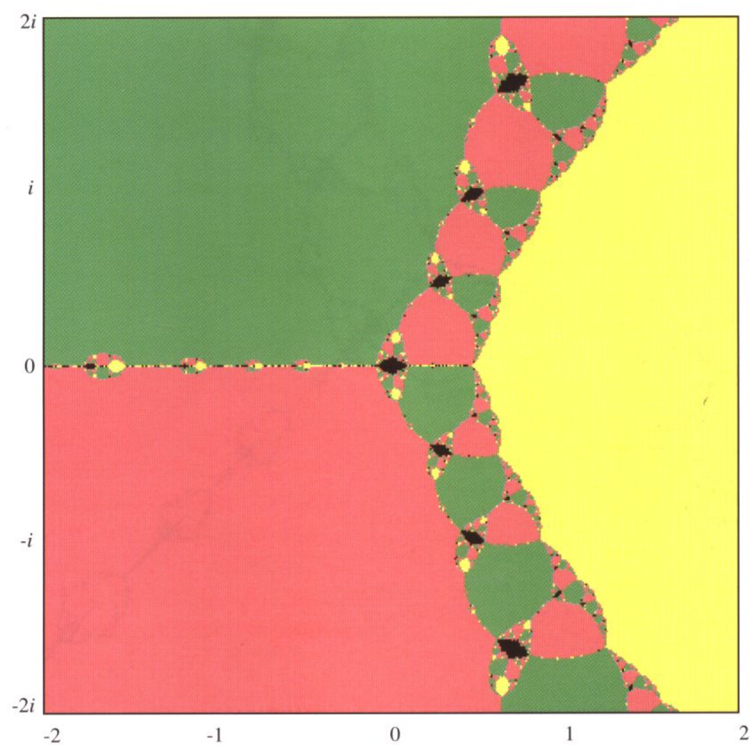

Fig. 3 Newton's method applied to $g(z) = (z-1)(z+0.5-0.33i)(z+0.5+0.33i)$. Note the black regions where the method fails.

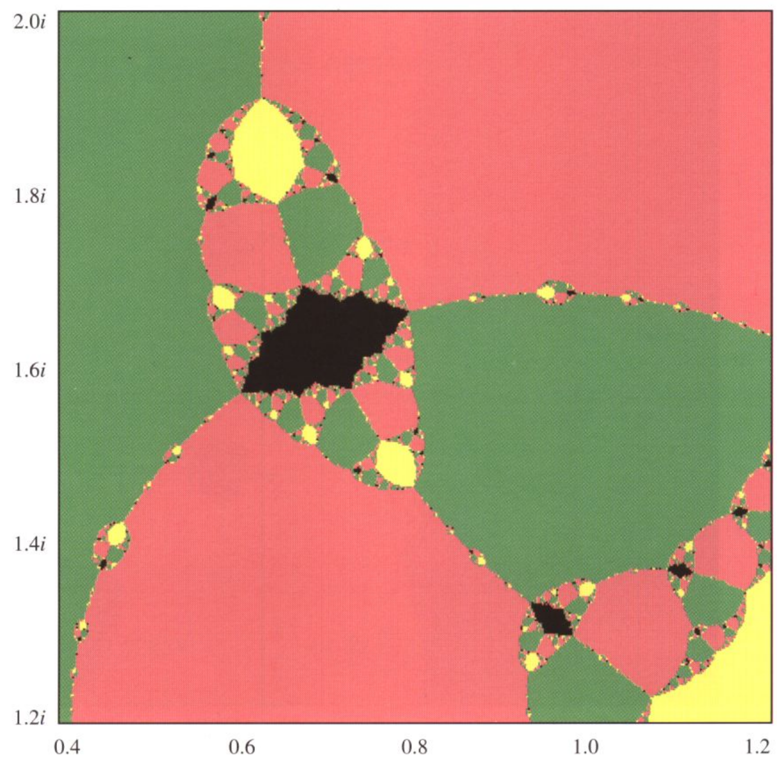

Fig. 4 A magnification of Fig. 3.

nomial g is a fixed point of N. A simple root is always super-attractive, and so Newton's method converges quadratically at such roots. At a multiple root of order k, the eigenvalue is $(k-1)/k < 1$, and so the method only converges linearly there. The point at infinity is always a repelling fixed point with eigenvalue $d/(d-1) > 1$, where d is the degree of the polynomial g. Hence large values of z_n will tend to be pushed away from infinity.

We normally iterate Newton's method until the difference between successive approximations is less than some fixed value. For example, the black points in Fig. 1 are those initial values in the complex plane for which successive iterates are not within 0.0001 of each other after 13 iterations of Newton's method for the cubic polynomial $g(z) = z^3 + iz - 1 - i$. This is an approximation to the Julia set of N. Figure 2 shows the basins of attraction for the roots 1, $-i$ and $-1+i$. Each white or colored region in Figs. 2–12 represents one basin of attraction of a root of g, while any points, whose iterates have not come sufficiently close to a root after a certain number of iterations, are colored black.

Figure 3 shows an example of Newton's method in which a whole neighborhood of initial points do not converge to any root. The points in the black regions converge to an attractive cycle of period 2 on the real axis. Hence Newton's method will fail for initial points in these black regions. A magnification of one of these regions is shown in Fig. 4.

4. RELAXED NEWTON'S METHOD

Because Newton's method is only linearly convergent at multiple roots, various modifications have been suggested for improving the convergence. If we know that g has a multiple root of order exactly m, we can apply Newton's method to $\sqrt[m]{g(z)}$ to obtain

$$N_m(z) = z - \frac{g(z)^{\frac{1}{m}}}{\frac{1}{m}\, g(z)^{\frac{1}{m}-1} g'(z)} = z - \frac{mg(z)}{g'(z)}.$$

This is called the *relaxed Newton's method* or *Newton's method for a root of order m*. This relaxed Newton's method will converge quadratically to a

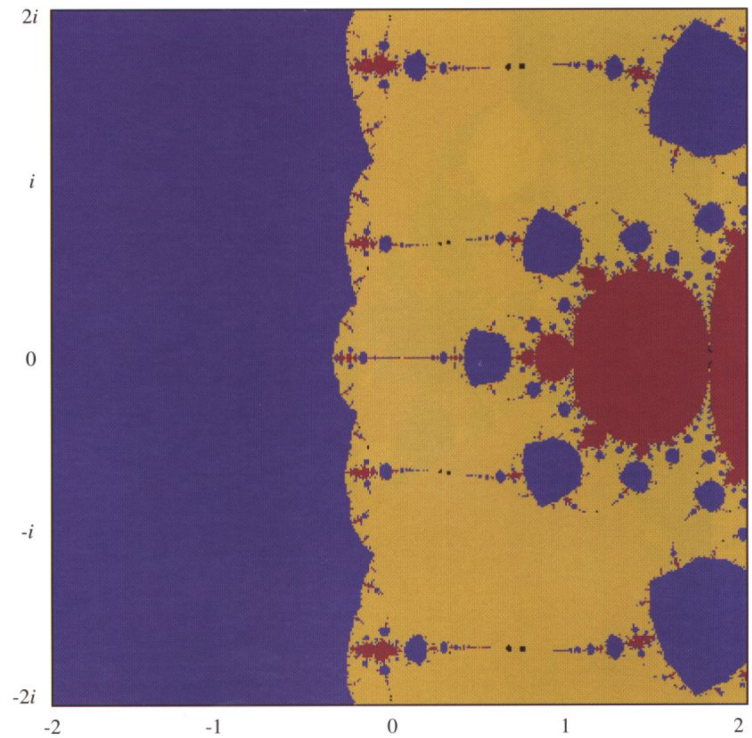

Fig. 5 The relaxed Newton's method applied to $g(z) = z(z-1)(z+1)^2$ using 1500 iterations.

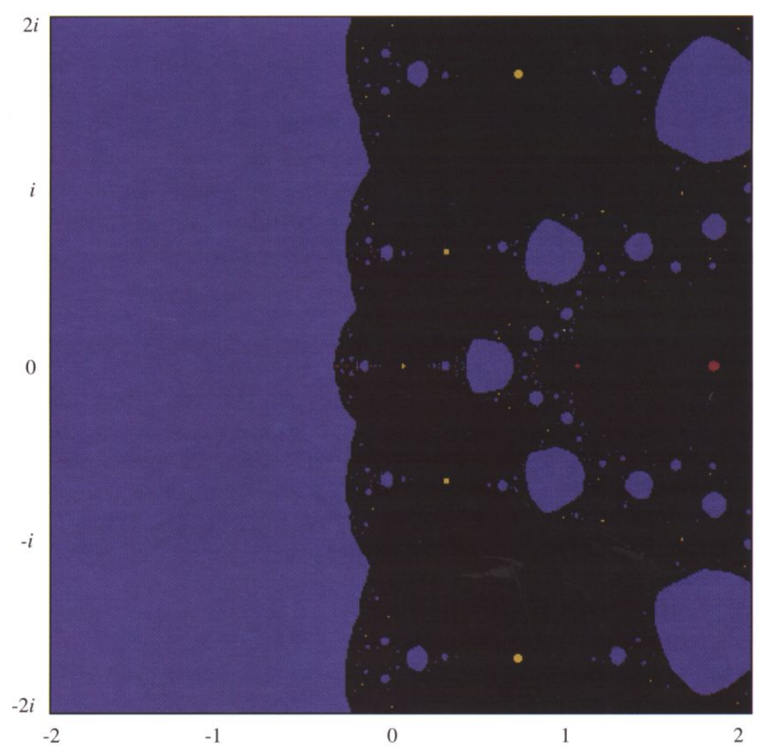

Fig. 6 The relaxed Newton's method applied to $g(z) = z(z-1)(z+1)^2$ using only ten iterations.

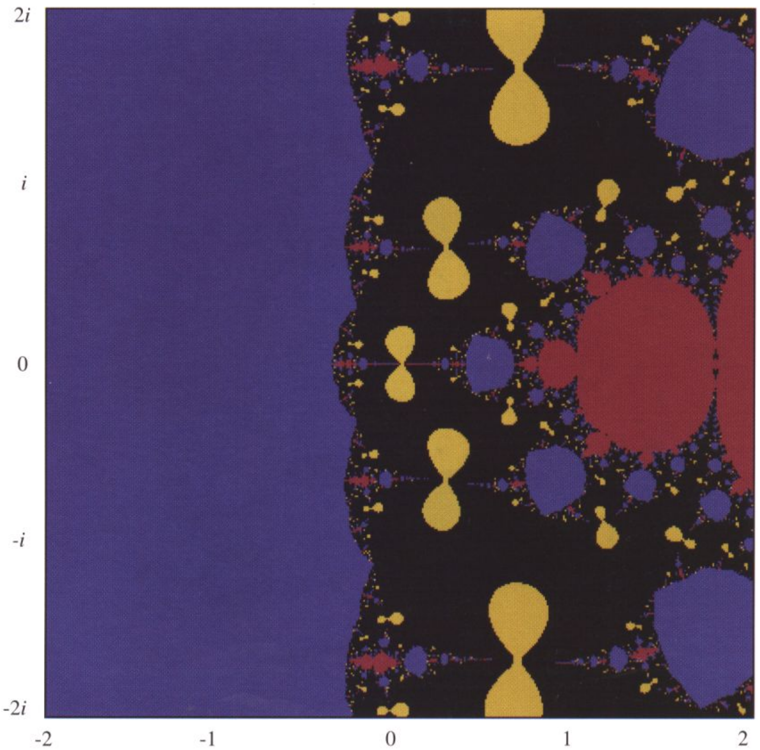

Fig. 7 The relaxed Newton's method applied to $g(z) = z(z-1)(z+1)^2$ using 1250 iterations.

root of order exactly m. At a root of order k, N_m has an eigenvalue of $1 - (m/k)$. If $m > 2k$, then $|1 - (m/k)| > 1$ and the root will be repelling. If $m < 2k$, then $|1 - (m/k)| < 1$ and the convergence will only be linear. If $m = 2k$, then the root is a neutral fixed point. The point at infinity is a repelling fixed point with eigenvalue $d/(d-m)$, where d is the degree of the polynomial g.

For example, it can be shown that the dynamics of the relaxed Newton's method N_2, applied to any cubic with one double root, is conjugate to the dynamics of the quadratic $p(z) = z^2 - \frac{3}{4}$.[10] The Julia set of this quadratic is well known. The simple root of such a cubic is a neutral fixed point for N_2, and points in its basin of attraction converge extremely slowly to the root.

Figure 5 shows the relaxed Newton's method N_2 applied to the quartic $g(z) = z(z-1)(z+1)^2$. The double root at -1 is super-attractive, but both simple roots at 0 and 1 are neutral fixed points, and it needed 1500 iterations for the colored points in the figure to converge to within 0.01 of these roots. If we only use ten iterations, as shown in Fig. 6, then points in the mauve region do converge to the double root, but very few points have come close to the simple roots. After 1250 iterations, shown in Fig. 7, the maroon basin of attraction of the simple root 1 is clear, but the yellow basin of attraction of the origin is not yet clearly defined. Therefore this relaxed method should only be tried if you are certain that you know the order of the multiple root, and you are in the basin of attraction.

The relaxed Newton's method can also be applied for non-integral values of m; in particular, see Refs. 11– 13 for results when $0 < m < 1$.

5. NEWTON'S METHOD FOR A MULTIPLE ROOT

If $g(z)$ is a polynomial with simple or multiple roots, then the rational function $g(z)/g'(z)$ will have a simple root for each root of $g(z)$. Apply Newton's method to $g(z)/g'(z)$ to obtain

$$M(z) = z - \frac{g(z)g'(z)}{g'(z)^2 - g(z)g''(z)}.$$

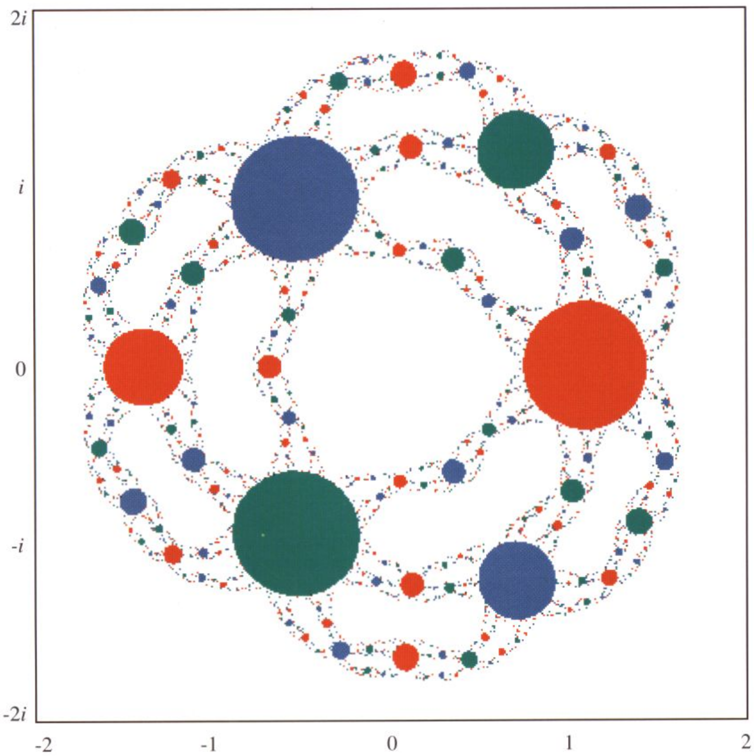

Fig. 8 Newton's method for a multiple root applied to $g(z) = z^2(z^3 - 1)$.

This is called *Newton's method for a multiple root.* It is quadratically convergent at every root of $g(z)$, but it is more complicated to calculate because it involves second derivatives.

The roots of $g(z)$ are not the only fixed points of $M(z)$. The roots of $g'(z)$, that are also not roots of $g(z)$, are extraneous fixed points for this method. However if w is such an extraneous fixed point, then $g'(w) = 0$, $g(w) \neq 0$ and $M'(w) = 2$. Therefore these extraneous fixed points are always repelling. This method $M(z)$ is the only one that we consider in which infinity is not a fixed point.

Figure 8 shows the method M applied to $g(z) = z^2(z^3 - 1)$ with one double root and three simple roots.[14]

6. COLLATZ METHOD

Collatz (Ref. 15, Sec. 17.5) shows that if we take the average of the relaxed Newton's method N_m, and Newton's method for a multiple root M, we obtain an iteration procedure that is cubically convergent at a root of order exactly m.

$$C_m(z) = \frac{N_m(z) + M(z)}{2}$$

$$= z - \frac{g(z)[(m+1)g'(z)^2 - mg(z)g''(z)]}{2g'(z)[g'(z)^2 - g(z)g''(z)]}\,.$$

If w is a root of $g(z)$ of order k, then

$$C'_m(w) = \frac{N'_m(z) + M'(z)}{2} = \frac{k - m}{2k}\,.$$

Hence, if $m > 3k$, the root will be repelling, if $m < 3k$ but $m \neq k$, the convergence will be linear and, if $m = 3k$, the root is a neutral fixed point. Any solutions to $(m+1)g'(z)^2 - mg(z)g''(z) = 0$, that are not roots of $g(z)$, are extraneous roots for this method. They should be checked to see if they are attractive or not. The point at infinity is always a repelling fixed point with eigenvalue $2d/(d - m)$, where d is the degree of the polynomial g.

Figure 9 shows the basins of attraction for the Collatz method, C_2, applied to the polynomial $g(z) = (2z + 1)^2(16z^3 + 24z^2 + 3)$. The convergence is cubic at the double root -0.5, and linear

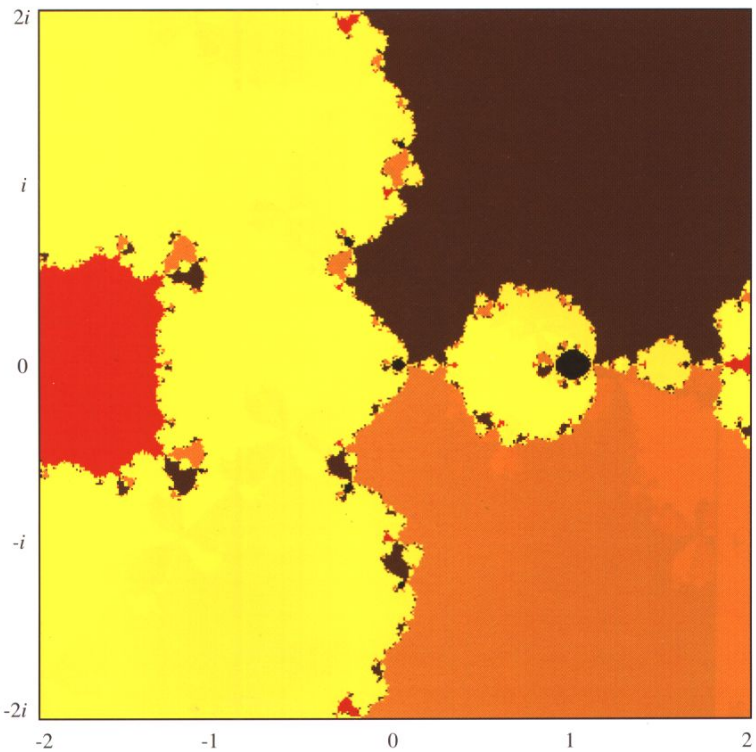

Fig. 9 The Collatz method applied to $g(z) = (2z+1)^2(16z^3+24z^2+3)$. Note the small black regions where the method fails.

at the other three roots. However, this example has a super-attractive extraneous fixed point at 0, and all points in the black regions converge to 0 rather than to any root.

7. SCHRÖDER METHOD

Schröder and König both produced modifications of Newton's method that will converge to any given order at a simple root. Let z_n be an approximation to a simple root of $g(z)$ in a neighborhood where the derivative $g'(z)$ is nonzero. We can approximate $y = g(z)$ by the polynomial $z = h(y) = a_0 + a_1 y + a_2 y^2 + \cdots + a_{r-1} y^{r-1}$, so that the two curves agree at z_n up to their $(r-1)$ derivatives. The curve $z = h(y)$ meets the z-axis at a_0, and we take this point to be the next approximation, z_{n+1}, to the root. This defines the *Schröder iteration method of the rth order*, $S_r(z)$ (Ref. 16, Sec. 3.34).[17] The Schröder method, S_r, converges to a simple root with order r. When $r = 2$, we are approximating the curve by the tangent at z_n, and so S_2 is just the standard Newton's method N. When $r = 3$, the method is defined by

$$\begin{aligned} S_3(z) &= z - \frac{g(z)}{g'(z)} - \frac{g''(z)g(z)^2}{2g'(z)^3} \\ &= z - \frac{g(z)[(2g'(z)^2 + g(z)g''(z)]}{2g'(z)^3}. \end{aligned}$$

The Julia sets associated with the Schröder method have been studied in Ref. 17.

At a root of order k, the eigenvalue for S_3 is $(k-1)(2k+1)/(2k^2)$ and so S_3 converges linearly at a multiple root. Extraneous fixed points of this method are solutions to $2g'(z)^2 + g(z)g''(z) = 0$, that are not roots of $g(z)$. The point at infinity is always a repelling fixed point for S_3 with eigenvalue $2d^3/(2d^3 - 3d^2 + d) > 1$, where d is the degree of the polynomial g.

Figure 10 illustrates the Schröder method, S_3, when it is applied to the same cubic polynomial $g(z) = (z-1)(z+i)(z+1-i)$ that was used in Figs. 1 and 2.

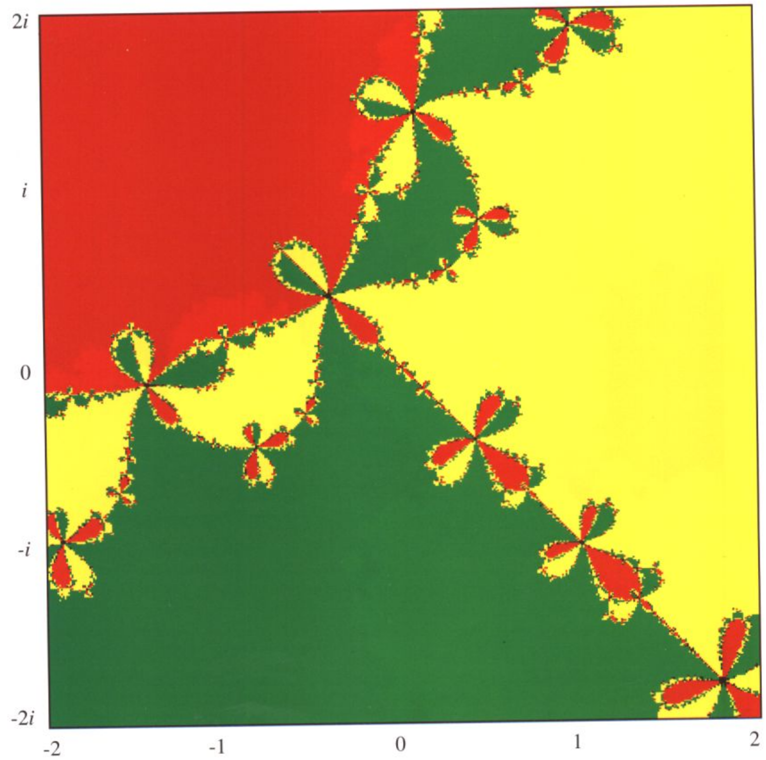

Fig. 10 Schröder's method applied to $g(z) = (z-1)(z+i)(z+1-i)$.

8. KÖNIG METHOD

If we apply Newton's method to $g(z)h(z)$, where $h(z)$ is finite and nonzero at a simple root of $g(z)$, then the resulting iteration will always be at least of second order at that simple root. In the *König iteration method of the rth order*, $K_r(z)$ (Ref. 16, Sec. 3.32), the function h is chosen so the iteration converges with order r at a simple root of g. K_2 is just the standard Newton's method. K_3 must satisfy $K_3''(w) = 0$ at a simple root w of $g(z)$, and we can take $h(z) = 1/\sqrt{g'(z)}$. K_3 is defined by

$$K_3(z) = z - \frac{2g(z)g'(z)}{2g'(z)^2 - g(z)g''(z)}\,.$$

This method, K_3, is also called the *Halley method.*[18]

At a root of order k, the eigenvalue for K_3 is $(k-1)/(k+1)$, and so K_3 converges linearly at a multiple root. The only extraneous fixed points of K_3 are roots of $g'(z)$ that are not roots of $g(z)$. These extraneous fixed points are all repelling.[19] The point at infinity is always a repelling fixed point for K_r with eigenvalue $(d+r-2)/(d-1)$, where d is the degree of the polynomial g.

Figure 11 shows the König method, K_3, when applied to the same cubic polynomial $g(z) = (z-1)(z+i)(z+1-i)$ that was used in Figs. 1, 2 and 10.

9. STEFFENSEN'S METHOD

The Steffensen method does not require the calculation of derivatives and only uses one initial value. The method may be derived from Aiken's process that is used to speed up the convergence of a sequence.[20] To find the roots of the function $g(z)$ we iterate

$$\mathrm{St}(z) = z - \frac{g(z)^2}{g(g(z)+z) - g(z)}\,.$$

If the denominator $g(g(z)+z) - g(z)$ is zero, we set $\mathrm{St}(z) = z$ and halt the iteration. The method converges quadratically at a simple root and linearly at multiple roots.

However, Fig. 12 shows that many initial points do not converge to any root. For any polynomial,

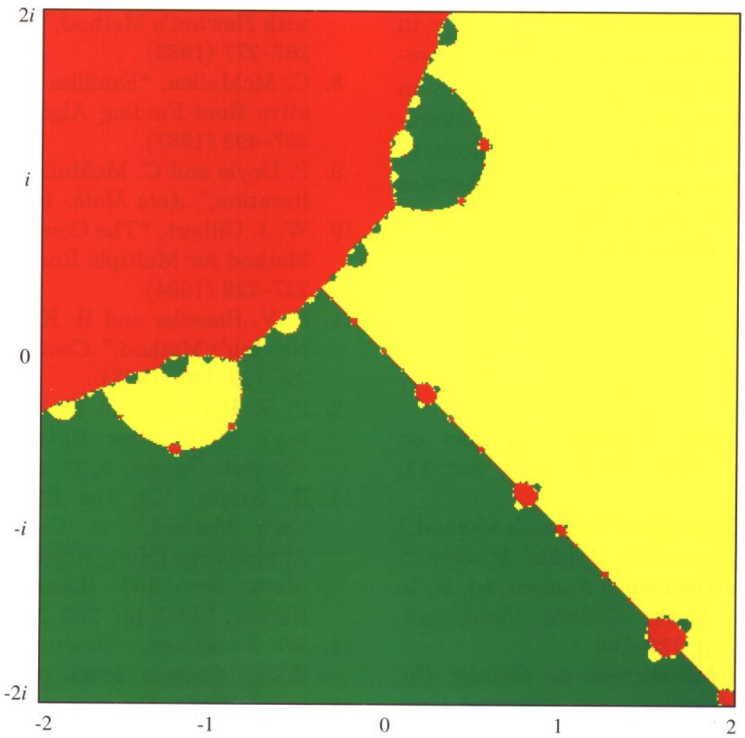

Fig. 11 König's method applied to $g(z) = (z - 1)(z + i)(z + 1 - i)$.

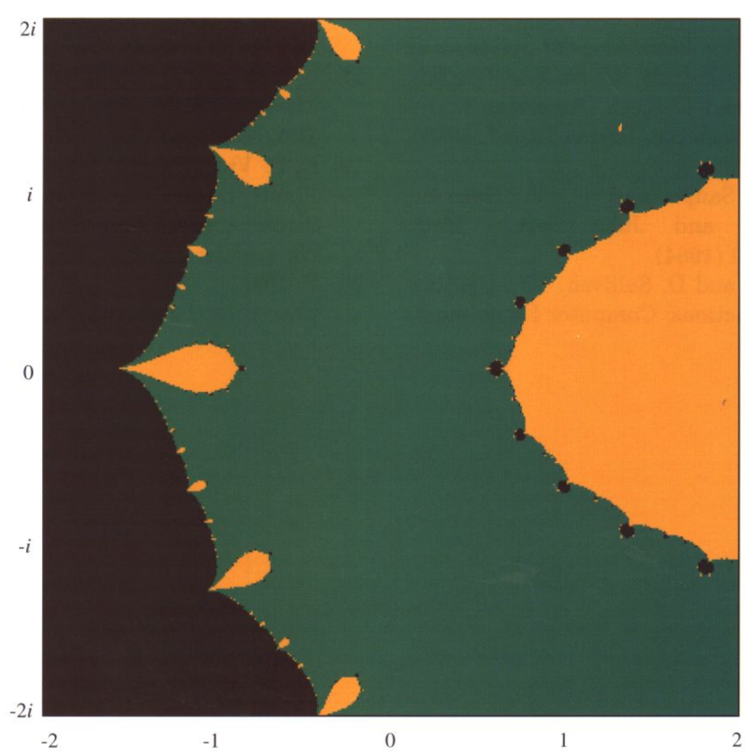

Fig. 12 Steffensen's method applied to $g(z) = z^2 - z$.

infinity is a neutral fixed point of $\mathrm{St}(z)$, while in most of our previous examples, infinity was a repelling fixed point. For initial starting values in the black regions, the iteration diverges. For example, if the initial value in Fig. 12 is a large positive real number in the yellow region, then the iterates will converge to 1. However, if the initial value is a large and negative real number, the iterates will slowly diverge.

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