



ISSN Print: 2394-7500
 ISSN Online: 2394-5869
 Impact Factor: 3.4
 IJAR 2015; 1(3): 129-134
 www.allresearchjournal.com
 Received: 20-12-2014
 Accepted: 22-01-2015

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Newton's method and voronoi diagram

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Abstract

Polynomial root finding is the origin of some fundamental discoveries in Mathematics and sciences. Where analytical or exact method fails, numerical approximation methods often succeed. We will investigate the numerical root finding method of Newton from a dynamical system perspective. Consider a complex valued function f and pick x_0 in the domain of f . If we iterate this function around x_0 , then we have sequence $x_0, f(x_0), f^2(x_0), \dots$ which becomes a dynamical system. We are essentially interested in the long term behavior of this system. We address the connection between behavior of both Newton's and Halley's methods with Voronoi diagram of underlying polynomial roots.

Keywords: Newton's method, Voronoi diagram

1. Introduction

It is usual to reduce a problem's solution to find roots of an equation in the science research and practical engineering. Now it has been proved theoretically that for a general polynomial equation of degree higher than 5, there is no analytic solution. Moreover, there is no root-finding algorithm formula to use for a general transcendental equation. In this case, it is much more important to study the numerical solution of non linear equations. Hence, iterative root-finding algorithms constitute one of the most important classes of iterative processes in mathematical applications. Newton's method is one of the most accessible and most easiest to implement of the iterative root-finding algorithm. It has quadratic convergence in the sense that sufficiently close to simple root each iteration of Newton's method will approximately double the number of correct decimal digits in a root approximation.

Here, we look at Newton's root-finding algorithm and discuss some of its properties. Also, we look at the relation between the basin of attraction of roots of a polynomial with respect to Newton's method and Voronoi diagram of the roots. Before moving forward, let us try to understand some basic concepts.

2. Preliminaries

2.1 Voronoi Diagram

There is a vast literature about Voronoi Diagrams and their applications continue to grow. A particularly notable use of a Voronoi Diagram was the analysis of the 1854 Cholera epidemic in London, in which Physician John Snow determined a strong correlation of deaths with proximity to a particular (infected) water pump.

If we start with a set of n distinct points, also called sites, (p_1, p_2, \dots, p_n) in the Euclidean plane, then their Voronoi diagram partitions the plane into convex sets $V(p_1), V(p_2), \dots, V(p_n)$. Here $V(p_i)$ is the set of all the points in the plane that are closer to p_i than to any other p_j . More precisely,

$$V(p_i) = \{z \in \mathbb{R}^2 : d(z, p_i) < d(z, p_j) \text{ for all } i \neq j\}$$

where d is the usual Euclidean metric on \mathbb{R}^2 . The set $V(p_i)$ is called the Voronoi cell of site p_i . The line segments which form the boundaries of Voronoi cells are called Voronoi edges. The endpoints of these edges are called Voronoi vertices.

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As is clear from the figure, the points on the Voronoi Edges are equidistant to two nearest sites and the Voronoi vertices are equidistant to three or more sites. Each Voronoi cell is a convex polygon.

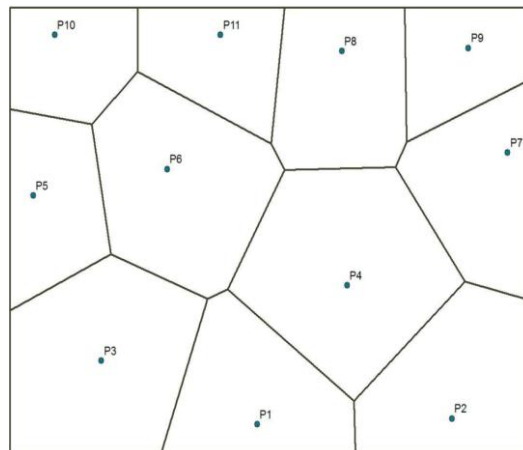


Fig 1: Voronoi diagram

2.2 Definitions

The problem of finding roots of polynomials has been the center of attraction in mathematical thinking since ages. At times, finding roots of a polynomial analytically is not possible. So new and different methods are developed to approximate roots. Some of these methods on which we will focus are based on iterations of rational functions. A function $f(z)$ is called a rational function if it can be written in the form $f(z) = \frac{P(z)}{Q(z)}$ where P and Q are polynomials with complex coefficients and Q is not the zero polynomial. Henceforth, we will be dealing with these kind of polynomials.

We are interested in the repeated application or iteration of a rational function $R(z)$. Specifically, we start with a point z_0 in the complex plane and then apply the rational map $R(z)$ repeatedly generating the points $z_0, z_1 = R(z_0), z_2 = R^2(z_0) \dots$ which brings us to our next definition.

Definition 1 (Orbit). Let $R(z)$ be a rational function. Consider the iteration $z_{k+1} = R(z_k), k = 0, 1, 2, \dots$, where z_0 is the starting point. Then the sequence $\{z_k\}_{k=0}^{\infty}$ is called the orbit of $R(z)$ at z_0 .

Many questions now present themselves; for example; does the sequence $\{z_n\}$ converges, or better still, for which values of the initial point z_0 , does the sequence converge? We will address these questions for some particular rational functions $R(z)$ in the later sections.

Definition 2 (Fixed Point). A point ζ is called a fixed point for a rational function R if $R(\zeta) = \zeta$

Classification of Fixed points

Let ζ be a fixed point of a function $R(z)$. Then ζ is

- a super-attracting fixed point if $|R'(\zeta)| = 0$.
- an attracting fixed point if $|R'(\zeta)| < 1$.
- a repelling fixed point if $|R'(\zeta)| > 1$.
- an indifferent fixed point if $|R'(\zeta)| = 1$.

Lemma 1. Let $R(z)$ be a rational function and (z_n) be the orbit of R starting at z_0 . If $z_n \rightarrow \omega$, then w is a fixed point of $R(z)$.

Definition 3 (Root finding Algorithm). We say that a map $f \rightarrow R_f$ carrying a complex-valued function f to another complex-valued function $R_f: \mathbb{C} \rightarrow \mathbb{C}$ is a root finding algorithm if R_f has a fixed point at every root of f and given an initial point $z_0 \in \mathbb{C}$, the iterates $(z_n)_0^{\infty}$ where $z_{k+1} = R_f(z_k)$ converge to a root $r \in \mathbb{C}$ of f whenever z_0 is sufficiently close to root of f .

One important parameter that determines the work accomplished per iteration is the order of convergence of the algorithm.

Definition 4 (Order of convergence). If there exists a constant $c \in \mathbb{R}, c > 0$ and a real number $k \geq 1$ such that $|z_{n+1} - r| \leq c |z_n - r|^k$ as $n \rightarrow \infty$ whenever z_0 is sufficiently close to any simple root of $r \in \mathbb{C}$ of f , then the method is said to be of order k convergent.

Definition 5 (Basin of Attraction). The basin of attraction of an attracting fixed point, ζ , of $R(z)$ is defined to be the set of all points z_0 in \mathbb{C} such that $R^n(z_0) \rightarrow \zeta$. It is denoted by $A(\zeta)$. In symbols, $A(\zeta) = \{z \in \mathbb{C} : R^n(z_0) \rightarrow \zeta\}$.

The rational maps of degree one are the Mobius maps $f(z) = \frac{az+b}{cz+d}$ where $ad - bc \neq 0$. Using these Mobius maps, we define an equivalence relation on the Rational maps.

Definition 6 (Conjugacy). We say that two rational maps R and S are conjugate if and only if there exists a Mobius map g such that $S = gRg^{-1}$

Properties of conjugacy

- If R and S are conjugate, then $\deg(R) = \deg(S)$.
- Conjugacy respects iteration: that is, if $S = gRg^{-1}$, then $S^n = gR_n g^{-1}$. This means we can transfer a problem concerning R to a problem concerning a conjugate S of R and then attempt to solve this in terms of S , which turns out to be very useful at times.
- Conjugacy respects fixed points. : explicitly, if $S = gRg^{-1}$, then S fixes $g(z)$ if and only if R fixes z .

Lemma 2. Every quadratic polynomial $f(z) = az^2 + bz + d$, $a \neq 0$, is conjugate by $s(z) = az + \frac{b}{2}$ to $fc(z) = z^2 + c$ where $c = ad + \frac{b}{2} - \frac{b^2}{4}$

Lemma 3. Every cubic polynomial $f(z) = z^3 + bz^2 + cz + d$, is conjugate by $h(z) = z + \frac{b}{3}$ to $g(z) = z^3 + pz + q$.

3. Newton’s Method

Newton’s method, probably the oldest and most famous iterative processes to be found in mathematics, can be used to approximate both real and complex solutions to the equation $f(z) = 0$.

3.1 Properties of Newton’s Method

Let $f(z)$ be any polynomial. We wish to solve $f(z) = 0$ using Newton’s method. It is an iterative method and is given by,

$$z_{k+1} = z_k - \frac{f(z_k)}{f'(z_k)}, k = 0, 1, 2, \dots$$

where z_0 is the starting point. Defining $N(z) = z - \frac{f(z)}{f'(z)}$, we see that it is a rational function and Newton’s Method deals with its repeated application.

$$N(z) .$$

Definition 7 (Multiplicity). Let $p(z)$ be a polynomial of degree n with complex coefficients. We say a $\epsilon \in \mathbb{C}$ is a root of $p(z)$ of multiplicity k if there exists a polynomial $g(z)$ such that $g(a) \neq 0$ and $p(z) = (z - a)^k g(z)$.

Theorem 4. Let $f(z)$ be a polynomial of degree $d \geq 2$. Let z^* be a root of f with multiplicity $m \geq 1$. Then z^* is an attractive fixed point of $N(z)$.

Proof. Since z^* is a root of f with multiplicity m , $f(z)$ can be written as

$$f(z) = (z - z^*)^m g(z)$$

where $g(z)$ is analytic at z^* and $g(z^*) \neq 0$. We evaluate $N(z)$.

$$\begin{aligned} N(z) &= z - \frac{f(z)}{f'(z)} \\ &= z - \frac{(z - z^*)^m g(z)}{m(z - z^*)^{m-1} g(z) + (z - z^*)^m g'(z)} \\ &= z - \frac{(z - z^*) g(z)}{m g(z) + (z - z^*) g'(z)} \end{aligned}$$

Observe that $N(z^*) = z^* - \frac{0}{g(z^*)}$. As $g(z^*) \neq 0$, we have $N(z^*) = z^*$ i.e. z^* is a fixed point of $N(z)$.

To show that z^* is an attracting fixed point, we need to find $|N'(z^*)|$. Since

$$N^1(z) = 1 - \left[\frac{(z - z^*)g(z)}{(z - z^*)g(z) + mg(z)} \right]^1$$

$$= 1 - \frac{(z - z^*)^2 \{g(z)\}^2 - (z - z^*)^2 g(z)g''(z)}{\{(z - z^*)g(z) + mg(z)\}^2}$$

$N'(z^*) = 1 - \frac{1}{m} < 1$. Thus z^* is an attractive fixed point of $N(z)$.

Theorem 5. A point z^* is a super-attracting fixed point of $N(z)$ if and only if z^* is a simple root of $f(z)$.

Proof. First, let z^* is a simple root of $f(z) = 0$. In the terminology of previous theorem we have $m = 1$. Thus, $N'(z^*) = 1 - 1 = 0$ which implies that z^* is a super-attracting fixed point of N .

Conversely, let z^* be a super-attracting fixed point of $N(z)$. Then,

$$N(z^*) = z^* \frac{f(z^*)}{f'(z^*)} = z^* \text{ implies } f(z^*) = m \cdot 0 \text{ i.e. } z^* \text{ is a root of } f \text{ of say multiplicity } m. \text{ Now by previous theorem and}$$

by the given condition that z^* is a super-attractive fixed point, $N'(z^*) = 1 - \frac{1}{m} = 0 \implies m = 1$. Thus z^* is a simple root of $f(z)$.

3.2 Newton's Method for quadratic polynomials

Theorem 6. For a quadratic polynomial, the basin of attraction of each root with respect to Newton's Method coincides with the Voronoi cell of the root.

Proof. Let $f(z)$ be the given polynomial. If f has a single root with multiplicity 2, then the result is obvious.

Let $f(z) = (z - \alpha)(z - \beta) = z^2 - (\alpha + \beta)z + \alpha\beta$ then $z = \alpha$ and $z = \beta$ are the roots of $f(z)$. Our aim is to show that $A(\alpha) = V(\alpha)$ and $A(\beta) = V(\beta)$.

Define $N(z)$ as

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

$$= z - \frac{z^2 - (\alpha + \beta)z + \alpha\beta}{2z - (\alpha + \beta)}$$

$$= \frac{z^2 - \alpha\beta}{2z - (\alpha + \beta)}$$

As we can see, $N(\alpha) = \alpha$ and $N(\beta) = \beta$. So $N(z)$ fixes both the roots of $f(z)$.

We start with a point in Voronoi cell of α and show that it belongs to the basin of attraction of α . For doing so, we define $g(z) = \frac{z - \alpha}{z - \beta}$. So the points which are nearer to α than to β are described as $\{ |g(z)| < 1 \}$. Then $g(\alpha) = 0$ and $g(\beta) = \infty$

Now we construct a rational function $R(z)$ conjugate to $N(z)$ as

$$R(z) = (gNg^{-1})(z) \text{ where } g(z) \text{ is as defined above and } g^{-1}(z) = \frac{\beta z - \alpha}{z - 1}$$

$$R(z) = (gNg^{-1})(z)$$

$$= (gNg^{-1})(z)$$

$$= (gN)\left(\frac{\beta z - \alpha}{z - 1}\right)$$

$$= g\left(\frac{\left(\frac{\beta z - \alpha}{z - 1}\right)^2 - \alpha\beta}{2\left(\frac{\beta z - \alpha}{z - 1}\right) - (\alpha + \beta)}\right)$$

$$= g\left(\frac{(\beta^2 - \alpha\beta)z^2 + (\alpha^2 - \alpha\beta)}{(\beta - \alpha)z^2 + (\alpha - \beta)}\right)$$

$$= g\left(\frac{\beta z^2 - \alpha}{z^2 - 1}\right)$$

$$\begin{aligned}
 &= \frac{\left(\frac{\beta z^2 - \alpha}{z^2 - 1}\right) - \alpha}{\left(\frac{\beta z^2 - \alpha}{z^2 - 1}\right) - \beta} \\
 &= \frac{(\beta - \alpha) z^2}{(\beta - \alpha)} \\
 &= z^2
 \end{aligned}$$

So finally we have $R(z) = z^2$. If we iterate R , we have $R^k(z) = (gN^k g^{-1})(z)$ which implies $N^k(z) = (g^{-1}R^k g)(z)$.

Let z_0 be a point in $V(\alpha)$. Then $|g(z_0)| < 1$ which implies $R^k(g(z_0)) \rightarrow 0$.

As $k \rightarrow \infty$, $N^k(z_0) \rightarrow g^{-1}(0) = \alpha$, $z_0 \in A(\alpha)$. Hence we have $V(\alpha) \subseteq A(\alpha)$ and if we trace the steps backward we will have $A(\alpha) \subseteq V(\alpha)$. So

$V(\alpha) = A(\alpha)$ and similarly we can prove the result for β , i.e. $V(\beta) = A(\beta)$

Let us first look at an example of a quadratic polynomial having a root with multiplicity 2. Let $f(z) = (z + 1)^2 = z^2 + 2z + 1$. Then $z = -1$ is a root of f with multiplicity 2.

Now consider $f_c(z) = z^2 + 1$, then the roots of $f_c(z)$ are $z = i - i$. Using MATLAB we plot the basin of attraction of the roots of these polynomials with respect to Newton's method. We observe that the basin of attraction of each root completely coincides with Voronoi cell of the root in both cases.

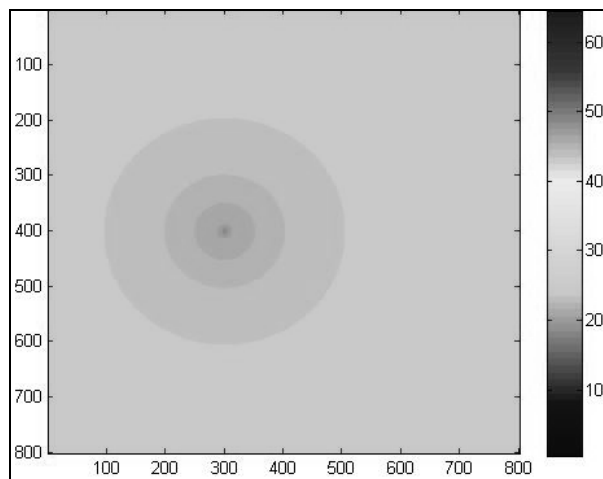


Fig 2: Basin of attraction of roots of $f(z) = (z + 1)^2$

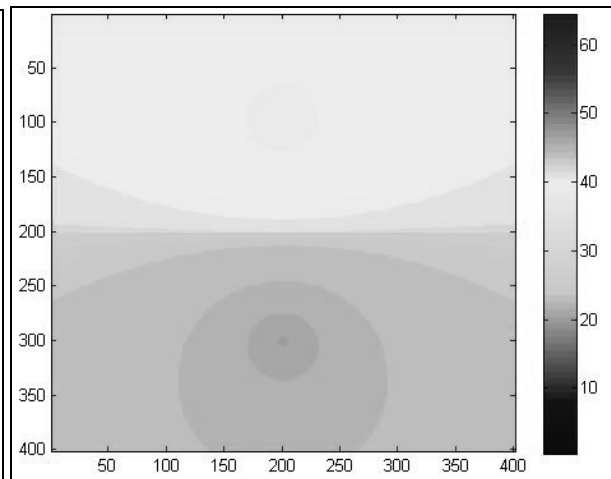


Fig 3: Basin of attraction of roots of $f_c(z) = z^2 + 1$

3.3 Newton's Method for cubic polynomials

We have seen the dynamics of Newton's method on quadratic polynomials but what happens to higher degree polynomials? As we will notice, the Voronoi cells provide a good approximation to the basin of attraction under Newton's method but the quality of this approximation varies with the degree of the polynomials. In this section we will look at the cubic polynomials.

Let us start with a cubic polynomial $p(z) = z^3 + c$. Then $p'(z) = 3z^2$.

$$\begin{aligned}
 N(z) &= z - \frac{p(z)}{p'(z)} \\
 &= z - \frac{z^3 + c}{3z^2} \\
 &= \frac{2z^3 - c}{3z^2}
 \end{aligned}$$

Let us plot the basin of attraction of roots for different values of c .

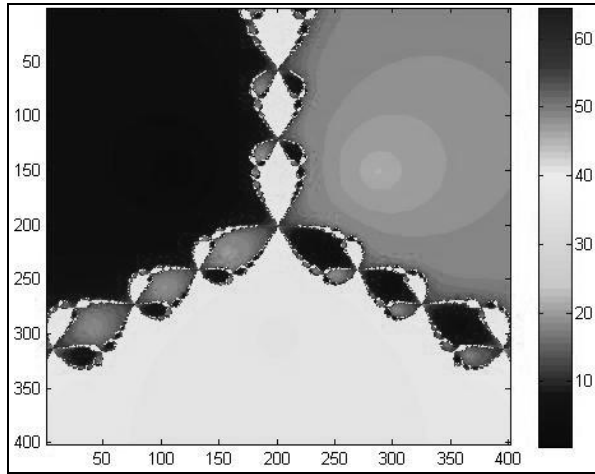


Fig 4: Basin for $N(z)$ when $f(z) = z^3 + i$

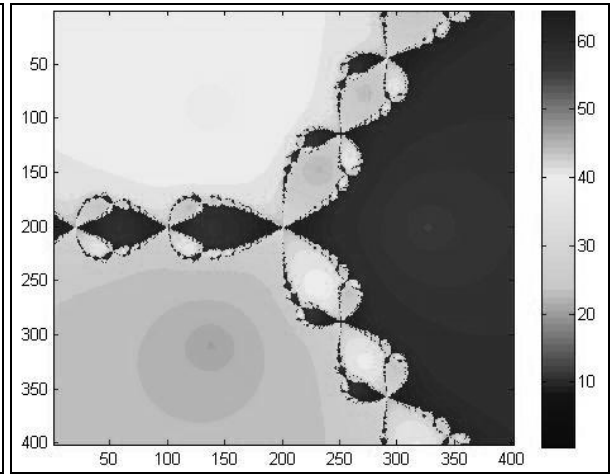


Fig 5: Basin for $N(z)$ when $f(z) = z^3 - 2$

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