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Voronoi diagram and Halley's method

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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 on the Riemann Sphere. For x_0 in the Sphere, we have sequence x_0, $f(x_0)$, $f^2(x_0)$, . . . which becomes a dynamical system. We are essentially interested in the long term behavior of this system. We address the connection between behavior of Halley's methods with Voronoi diagram of the roots of the underlying polynomial

Keywords: Voronoi diagram, Halley's method

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 iterative root-finding algorithm. It has quadratic convergence in the sense that for points sufficiently close to simple root each iteration of Newton's method approximately double the number of correct decimal digits in a root approximation.
[5] McMullen proved several important results about root-finding algorithms. First, he proved that there can be no generally convergent algorithm for polynomials of degree 4 and higher. In addition he gave an explicit formula for a generally convergent algorithm for cubic polynomials. Here, we look at Halley'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 these methods and Voronoi diagram of the roots.

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, . . . p_n) in the Euclidean plane, then their Voronoi diagram partitions the plane into convex sets V (p_1), V (p_2), . . . V (p_n). Here V (p_i) is the set of all the points in the plane that are closer to pi than to any other p_j. More precisely,

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

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.

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 [1, 3].

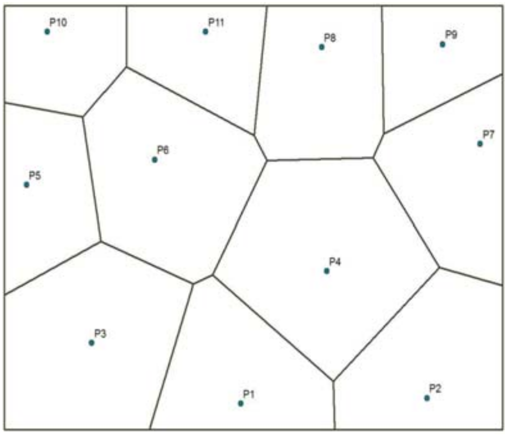

Fig 1: Voronoi diagram

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) ………….. 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 ………, 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 }converge, 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(* ζ *)=* ζ

Classification of Fixed points [4]

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

- A super-attracting fixed point if $|R^1(\zeta)| = 0$.
- An attracting fixed point if $|R^1(\zeta)| < 1$.
- A repelling fixed point if $|R^1(\zeta)| > 1$.
- An indifferent fixed point if $|R^1(\zeta)| = 1$.

Lemma 1. [4] *Let R(z) be a rational function and {z_n} be the orbit of R starting at z_0. If* $\lim_{n\to\infty} z_n \to \omega$*, then* ω *is a fixed point of R(z).*

Definition 3 *(Root finding Algorithm). We say that a map f* $\rightarrow$ *R_f carrying function f :* $\mathbb{C} \rightarrow \mathbb{C}$ *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 = Rf (zk) converge to a root r 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 of f, then the method is said to have order of convergence k.*

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 $\lim_{n \to \infty} R^n (z_0) = \zeta$. It is denoted by A ($\zeta$).

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 a 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 $S^n = gR_ng^{-1}$.

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 $f_c(z) = z^2 + c$ 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. Halley's Method

Halleys method is a root-finding algorithm used for functions with complex coefficients and having a continuous second derivative, i.e., C^2 functions. It is named after its inventor Edmond Halley. Halley is well known for first computing the orbit of the Halley comet. Halley generalized an iteration formula for computing the cube root of a number and obtained an iteration function to compute roots of the polynomial.

3.1 Properties of Halley's Method

Definition 7 (Halley's Method). Let $f(z)$ be any polynomial and define H (z)
As

$$H(z) = z - \frac{2 f(z) f^{1}(z)}{2 (f^{1}(z))^2 - f(z) f^{11}(z)}$$

The algorithm $z_n+1 = H(z_n)$, where z_0 is the starting point, is called Halley's method.

Theorem 4. Let f(z) be a polynomial of degree $d \geq 2$ and let z_0 be a root of $f(z)$ of multiplicity $m \geq 1$. Then z_0 is an attracting fixed point of H(z).

Proof. Let z_0 be a root of $f(z)$. Then

$$H(z) = z - \frac{2 f(z) f^{1}(z)}{2 (f^{1}(z))^2 - f(z) f^{11}(z)}$$ and $H(z_0) = z_0 - 0 = z_0$

Hence, z_0 is a fixed point of H (z). Now to show that z_0 is an attracting fixed point, first let us evaluate $H^1(z)$.

$$H^1(z) = 1 - 2 \left(\frac{f(z) f^{1}(z)}{2 (f^{1}(z))^2 - f(z) f^{11}(z)} \right)$$

$$= 1 - 2 \left[\frac{\{2 (f^{1})^2 - f f^{11}\} \{f f^{11} + (f^{1})^2\} - \{f f^{1}\} \{4 f^{1} f^{11} - f f^{111} - f^{1} f^{11}\}}{\{2 (f^{1})^2 - f f^{11}\}^2} \right]$$

$$= 1 - 2 \left[\frac{2 (f^{1})^4 - f^2 (f f^{11})^2 - 2 f (f^{1})^2 f^{11} + f^2 f^{1} f^{111}}{\{2 (f^{1})^2 - f f^{11}\}^2} \right]$$

Consider the polynomial $f(z)$. Let z_0 be a root of f(z) of multiplicity m $\geq$ 1.
Then $f(z)$ can be factored as $f(z) = (z - z_0)^m g(z)$ where $g(z_0) \neq 0$. We write $z - z_0 = k$ and $g(z) = g$ for simplicity. Then

$$f^1 = k^m g^1 + mk^{m-1} g = k^{m-1} (kg^1 + mg)$$

$$f^{11} = k^m g^{11} + 2mk^{m-1} g^1 + m(m-1)k^{m-2} g = k^{m-2} (kg^1 + mg)$$
$$f^{111} = k^{m-3} (k63g^{111} + 2mk^2 g^{11} + 3m(m-1)g^1 + m(m-1)(m-2)g)$$

Putting these values in $H^1(z)$ and evaluating $H^1(z)$ at $z = z_0$ i.e. at $k = 0$, we get

$$H^1(z_0) = 1 - \frac{2}{m+1} < 1$$

Hence z_0 is an attracting fixed point of H(z).

Example Let $f(z) = z^2 - 1$. Then the roots of $f(z)$ are $z = 1$ and $z = -1$.

Now $f^1(z) = 2z$ and $f^{11}(z) = 2$.

$$H(z) = z - \frac{2(z^2-1)(2z)}{2(2z)^2 - (z^2-1)(2)}$$

$$= z - \frac{4z^3 - 4z}{6z^2 + 2}$$

$$= \frac{2z^3 + 6z}{6z^2 + 2}$$

$$= \frac{z^3 + 3z}{3z^2 + 1}$$

Now $H(1) = 1$ and $H(-1) = -1$ which shows H fixes both the roots of f(z).
Now

$$H^1(z) = \frac{(3z^2+1)(3z^2+3) - (z^3+3z)(6z)}{(3z^2+1)^2}$$

$$= \frac{6z^4 - 6z^2 + 3}{(3z^2+1)^2}$$

$H^1(1) = 0$ and $H^1(-1) = 0$ which shows that $z = 1$ and $z = -1$ are super attracting fixed points of H(z).

Theorem 5. Let $f(z)$ be a polynomial of degree d $\geq$ 2 and let H(z) be the rational function as defined above. Then a point r is a super-attracting fixed point of H(z) if and only if r is a simple root of $f(z)$. Any other fixed point of H (z) is repelling. [6]
Proof. Let r be a simple root of $f(z)$. By previous theorem, r is an attracting fixed point of H(z). In the notation of the previous theorem, m = 1, i.e. multiplicity of r is 1. But $H^1(r)$

$= 1 - \frac{2}{m+1} = 1 - \frac{2}{2} = 0$. Hence r is a super attracting fixed point of H(z).

Conversely, let r be a super attracting fixed point of H(z) and we have to show that r is a simple root of f(z). By definition, $H(r) = r$ and $H^1(r) = 0$ which gives that $f(r) f^1(r) = 0$. So either $f(r) = 0$ or $f^1(r) = 0$. If $f(r) = 0$, then r is a root of f and by previous theorem, we know $H^1(r) = 1 - \frac{2}{m+1}$, where m is the multiplicity of r. $H^1(r) = 0$ gives m = 1. Hence r is a simple root of f. In the second case, let $f(r) \neq 0$ and $f^1(r) = 0$. Then r is a root of $f^1(z)$. Let j be its multiplicity. Then $f^1(z)$ can be factored as $f^1(z) = (z - r)^j g(z)$ where $g(r) \neq 0$. Now putting these values in $H^1(z)$, we get $H^1(r) = 1 + \frac{2}{j} > 1$. So we have r is a repelling fixed point in this case.

Example
In this example, we will illustrate that a fixed point of H(z) which is not a root of f is a repelling fixed point. Let $f(z) = z^3 + 1$, then $f^1(z) = 3z^2$ and $f^{11}(z) = 6z$.

$$H(z) = z - \frac{2(z^3+1)(3z^2)}{2(3z^2)^2 - (z^3+1)(6z)}$$

$$= z - \left(\frac{z^5+z^2}{2z^4+z}\right)$$

$$= \frac{z^5 - 2z^2}{2z^4 - 2}$$

For finding the fixed points of H(z), we have to solve H(z) = z.

$z^5 - 2z^2 = 2z^5 - z^2$

So the fixed points of H are the solutions of $z^2(z^3 + 1) = 0$. The only fixed point other than the roots of *f* is z = 0. We claim 0 is a repelling fixed point.

$$H^1(z) = \frac{(2z^4 - z)(6z^4 - 4z) - (z^4 - 2z^2)(8z^3 - 1)}{(2z^4 - 1)^2}$$

$$= 2\left(\frac{z^6 + 2z^3 + 1}{(2z^3 \quad 1)^2}\right)$$

Hence $H^1(0) = 2 > 1$, which implies that 0 is a repelling fixed point.

3.2 Halley's Method for quadratic polynomials

The dynamics of Halley's method for quadratic polynomials is very simple and is easy to understand.

Theorem 6. For a quadratic polynomial, the basin of attraction of each root with respect to Halley'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 $f(z) = (z - \alpha)(z - \beta) = z^2 (\alpha + \beta) z + \alpha \propto \beta$ and observe that $f^1(z) = 2z - (\alpha + \beta)$ and $f^{11}(z) = 2$. Therefore

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

$$= z - \left[\frac{z^3 - 3(\alpha+\beta)z^2 + ((\alpha+\beta)^2 + 2\alpha\beta)z - \alpha(\alpha+\beta))}{3z^2 - 3(\alpha+\beta)z + (\alpha+\beta)^2 - \alpha\beta}\right]$$

$$= \frac{z^3 - 3\alpha\beta z + \alpha\beta(\alpha+\beta)}{3z^2 - 3(\alpha+\beta)z + (\alpha+\beta)^2 - \alpha\beta}$$

Now defining $g(z) = \frac{z-\alpha}{z-\beta}$, note that $g(\alpha) = 0$ and $g(\beta) = 1$. Also $g^{-1}(z) = \frac{\beta z - \alpha}{z-1}$

Consider the rational function $R(z) = (gH g^{-1})(z) = (gH)\left(\frac{\beta z - \alpha}{z-1}\right)$

We first evaluate $H\left(\frac{\beta z - \alpha}{z-1}\right)$ which is

$$= \frac{\left(\frac{\beta z - \alpha}{z-1}\right)^3 - 3\alpha\beta\left(\frac{\beta z - \alpha}{z-1}\right) + \alpha\beta(\alpha+\beta)}{3\left(\frac{\beta z - \alpha}{z-1}\right)^2 - 3(\alpha+\beta)\left(\frac{\beta z - \alpha}{z-1}\right) + (\alpha|+\beta)^2 - \alpha\beta}$$

$$= \frac{(z-1)^3}{\frac{(\alpha-\beta)^3 z^3 + (\alpha+\beta)^3 z + (\alpha-\beta)^3}{(z-1)^3}}$$

$$= \frac{\beta z^3 - \alpha}{(z-1)(z^2+z+1)}$$

So $R(z) = \left(gH\left(\frac{\beta z-\alpha}{z-1}\right)\right) = g\left(\frac{\beta z^3-\alpha}{(z-1)(z^2+z+1)}\right) = z^3$

If we iterate R, we have $R^k(z) = (gH^kg^{-1})(z)$ which implies $H^k(z) = (g^{-1}R^kg)(z)$.

Let z_0 be a point in V (α). Then $|g(z_0)| < 1$ and $R^k(g(z_0)) \to 0$ as $k \to \infty$

As $k \to \infty$, $H^k(z_0) \to g^{-1}(0) = \alpha$ which implies $z_0 \in A(\alpha)$. 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. $V(\beta) = A(\beta)$

Now consider $f(z) = z^2 - 2$, then the roots of $fc(z)$ are $z = \sqrt{2}, -\sqrt{2}$ Using MATLAB we plot the basin of attraction of the roots of these polynomials with respect to Halley's method. We observe that the basin of attraction of each root completely coincides with Voronoi cell of the root.

3.3 Halley's Method for polynomials of higher degree

As we have seen in the case of Newton's method, the basin of attraction of roots of higher degree polynomials are not as simple looking as quadratic polynomials.

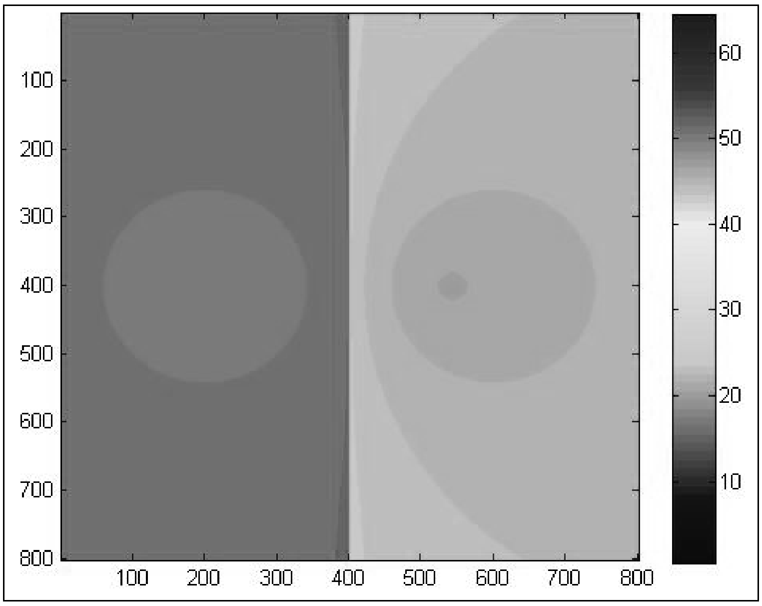

Fig 2: Basin for H(z) when $f(z) = z^2 - 2$

But still Halley's Method provides a slight improvement over Newton's method. First let's look at the cubic polynomial $f(z) = z^3 + c$. Then $f^1(z) = 3z^2$, $f^{11}(z) = 6z$ and

$$H(z) = z - \left[\frac{2(z^3+c)(3z^2)}{2(3z^2)^2 - 6z(z^3+c)}\right]$$

$$= z - \left[\frac{6z^5 + 6cz^2}{12z^4 - 6cz}\right]$$

$$= z - \left[\frac{z^5 + cz^2}{2z^4 - cz}\right]$$

Let's have a visual of the dynamics of this polynomial under Halley's method.

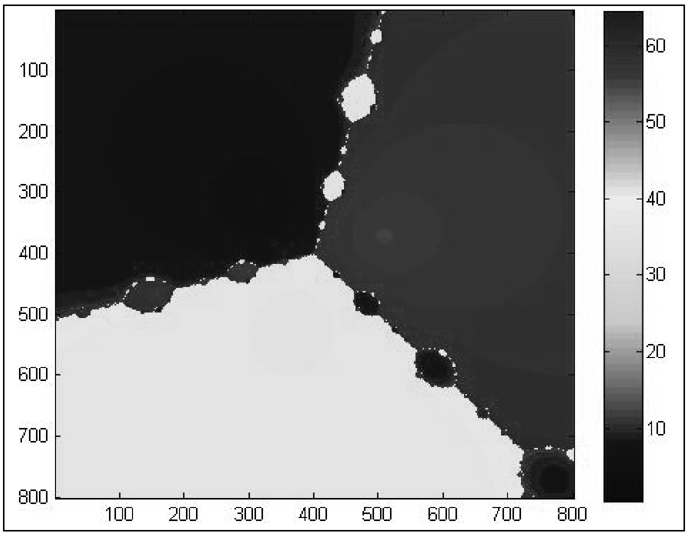

Fig 3: Basin for H(z) when $f(z) = z^3 + 1 - i$

Let $f(z) = z^3 + az + b$, then $f^1(z) = 3z^2 + a$ and $f^{11}(z) = 6z$. The Halley's method is

$$H(z) = z - \left[\frac{2(z^3 + az + c)(3z^2 + a)}{2(3z^2 + a)^2 - 6z(z^3 + az + c)}\right]$$

$$= z - \left[\frac{2(z^3 + az + c)(3z^2 + a)}{2(3z^2 + a)^2 - 6z(z^3 + az + c)}\right]$$

$$= z - \left[\frac{3z^5 + 4az^3 + 3bz^2 + a^2z + ab}{6z^4 + 3az^2 + (a^2 - 3bz)}\right]$$

Then the basin of attraction of roots of $f(z)$ are represented in the following figure. Now let's move one step ahead and look at a polynomial of degree 4.

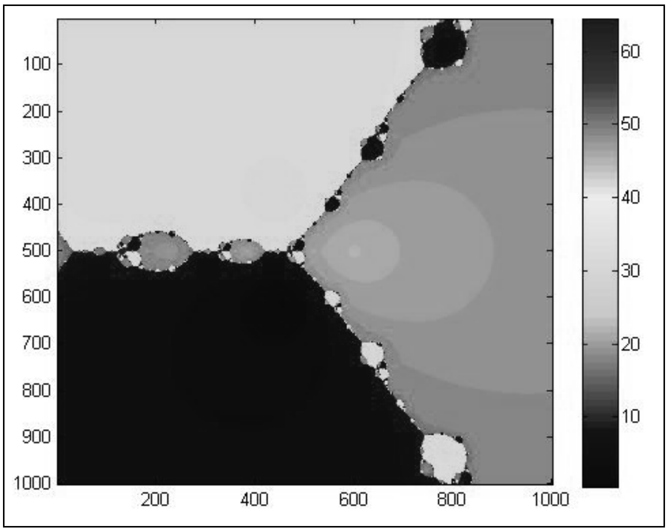

Figure 4: Basin for H(z) when $f(z) = z^3 + \frac{z}{2} - \frac{3}{2}$

Let $f(z) = z^4 + 1$, then $f^1(z) = 4z^3$ and $f^{11}(z) = 12z^2$. Then

$$H(z) = z - \frac{2(z^4+1)(4z^3)}{2(4z^3)^2 - (z^4+1)(12z^2)}$$

$$= z - \frac{8z^3(z^4+1)}{20z^6 - 12z^2}$$

$$= z - \frac{2z^5 + 2z}{5z^4 - 3}$$

The basin of attraction of roots of *f*(z) are represented in the following figure.

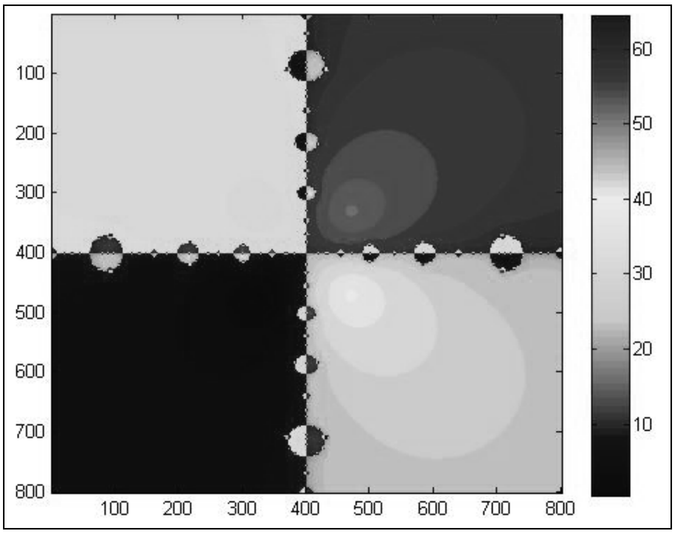

Fig 5: Basin for H(z) when *f*(z) = $z^4 + 1$

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