Halley’s Method as the First Member of an Infinite Family of Cubic Order Rootfinding Methods

Bahman Kalantari

Department of Computer Science
Rutgers University, New Brunswick, NJ 08903

Abstract

For each natural number $m \geq 3$, we give a rootfinding method $H_m$, with cubic order of convergence for simple roots. However, for quadratic polynomials the order of convergence of $H_m$ is $m$. Each $H_m$ depends on the input, the corresponding function value, as well as the first two derivatives. We shall refer to this family as Halley Family, since $H_3$ is the well-known method of Halley. For all $m \geq 4$, the asymptotic error constant of $H_m$ is the same constant. Each $H_m$ is described in terms of determinants that are computable recursively. The Halley Family and their derivative-free variants offer alternatives to the traditional rootfinding methods, such as secant, Newton, and Muller methods, as well as Halley’s method itself.

Keywords: Rootfinding, Halley’s Method, Order of Convergence.

AMS Subject Classification. 65H05.
1 Introduction.

In this paper we consider the rootfinding problem for smooth functions of a single variable. For each natural number $m \geq 3$, we give a rootfinding method $H_m$, cubically convergent for simple roots. We will refer to this family as Halley Family since its first member is the iteration function of the well-known method of Halley. To describe the family, for each $m \geq 1$, let $A_m(x)$ be the $m \times m$ matrix having the following properties: all its diagonal entries are $f'(x)$, all its subdiagonal entries are $f(x)$, all its superdiagonal entries are $f''(x)/2$, and all other entries are zero. Thus,

$$A_m(x) = \begin{pmatrix} f'(x) & \frac{f''(x)}{2} & 0 & \ldots & 0 \\ f(x) & f'(x) & \frac{f''(x)}{2} & \ddots & 0 \\ 0 & f(x) & f'(x) & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \frac{f''(x)}{2} \\ 0 & 0 & 0 & \ldots & f'(x) \end{pmatrix}.$$ 

Let

$$h_m(x) = \det(A_m(x)),$$

where $\det(\cdot)$ denotes the determinant. As we shall see $h_m(x)$ satisfies the recursion:

$$h_m(x) = f'(x)h_{m-1}(x) - \frac{1}{2} f(x)f''(x)h_{m-2}(x).$$

For each $m \geq 3$, define

$$H_m(x) = x - f(x) \frac{h_{m-2}(x)}{h_{m-1}(x)}.$$ 

The function

$$H_3(x) = x - f(x) \frac{f'(x)}{f'(x)^2 - \frac{1}{2} f(x)f''(x)}$$

is the iteration function of Halley’s method. The method was first considered by the astronomer Halley [7]. Halley’s method and its asymptotic error constant has been derived by many authors, see e.g. Alefeld [1], Bateman [2], Bodewig [3], Brown [4], Frame [5], Gander [6], Hamilton [8], Hansen and Patrick [9], Ostrowski [16], Popovski [17], Stewart [19], Traub [20], Wall [21], and [10]. For the interesting history of Halley’s method see Traub [20], Scavo and Thoo [18], and Ypma [22].

For all $m \geq 4$, the asymptotic error constant of $H_m$ is the same constant. However, for quadratic polynomials the order of convergence of $H_m$ is $m$. We will show that once we have evaluated $H_m$ at an input $x_0$, $H_{m+1}(x_0)$ can be computed in constant number of arithmetic operations, independent of $m$. These iteration functions and their derivative-free variants offer
alternatives to the traditional rootfinding methods, such as secant method and Newton’s methods which are based on linear approximation, Muller’s method which is a derivative-free method based on quadratic approximation, as well as Halley’s method itself.

Although the results of this paper are self-contained, the discovery of the Halley Family is the outgrowth of several nontrivial results. One of these results is the existence of a fundamental family of iteration functions, called the Basic Family, \( \{B_m(x)\}_{m=2}^\infty \), see [10], [11], and [13]. For simple roots the order of convergence of \( B_m(x) \) is \( m \). The Basic Family can be described in terms of a determinantal formula. Let \( U_{k+1}(x) \) be the \((k+1) \times (k+1)\) upper triangular matrix such that for each \( i = 1, \ldots, k+1 \), all its \( i \)-th diagonal entries are \( f^{(i-1)}(x)/(i-1)! \). Let \( D_k(x) \) be the determinant of the \( k \times k \) matrix that results after deleting the first column and the last row of \( U_{k+1}(x) \). Then,
\[
B_m(x) = x - f(x) \frac{D_{m-2}(x)}{D_{m-1}(x)}, \quad m \geq 2.
\]
In particular, each \( B_m(x) \) depends on the input \( x \), \( f(x) \), and its first \( m-1 \) derivatives. For each natural number \( t \) it is possible to define a family of iteration function \( \{B_{m,t}(x)\}_{m=t+1}^\infty \), where in \( B_m(x) \) we set all derivatives higher than the \( t \)-th derivative equal to zero. We shall refer to \( B_{m,t}(x) \) as the Truncated Basic Family of order \( t \). In the present paper we consider the special case of the Halley Family, \( \{H_m(x) \equiv B_{m,2}(x)\}_{m=3}^\infty \). We prove that each member has cubic order.

More generally, in a forthcoming paper, [15], we will show that each member of the family of iteration functions \( \{B_{m,t}(x)\}_{m=t+1}^\infty \) has order \( t + 1 \). An additional interesting property of the Truncated Basic Family is that for polynomials of degree at most \( t \), the order of \( B_{m,t}(x) \) is \( m \). This property is a direct consequence of the fact that \( B_m(x) \) has order of convergence equal to \( m \). Note that the family \( \{B_{m,1}(x)\}_{m=2}^\infty \) consists of a single element, namely Newton’s iteration function \( B_2(x) = x - f(x)/f'(x) \).

The Halley Family gives rise to the following rootfinding algorithm:

**Step 1.** Given an input \( x_0 \), let \( P_2(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2}(x - x_0)^2 \).

**Step 2.** Approximate a root of \( P_2(x) \) using the sequence \( \{H_m(x_0)\}_{m=3}^\infty \) according to:

- **Strategy I.** Let \( x_1 = H_3(x_0) \).

- **Strategy II.** Fix \( \epsilon > 0 \). Let \( x_1 = H_m(x_0) \), where \( m \) is the least \( m \geq 4 \) such that
\[
|H_m(x_0) - H_{m-1}(x_0)| \leq \epsilon.
\]

**Step 3.** Replace \( x_0 \) with \( x_1 \). Go to Step 1.

The above algorithm, if it only invokes Strategy I is simply Halley’s method. The justification in using Strategy II lies in the following result proved in [14]: if \( f \) is a polynomial with complex
coefficients, and \( \theta \) a simple root, there exists a neighborhood of \( \theta \) so that for any input \( x_0 \) in this neighborhood, we have

\[
\theta = \lim_{m \to \infty} B_m(x_0).
\]

In particular, if \( x_0 \) is a reasonably good approximation to a simple root \( \theta \) of \( P_2(x) \), then \( \theta = \lim_{m \to \infty} H_m(x_0) \). Thus, the above algorithm is an algorithm that obtains an approximation to a root of the quadratic Taylor polynomial at the current iterate, \( x_0 \), where this approximation is achieved via the Halley Family, all evaluated at \( x_0 \). For a more general version of this algorithm see [14].

It is possible to define multipoint versions of Halley’s method. These are special cases of the multipoint versions of the Basic Family described in Kalantari [13], and analyzed in Kalantari [12]. A version of Halley’s method can be defined using only the first derivatives, thus comparable with Newton’s method. However, its order of convergence is 2.41. Also, a derivative-free version of Halley’s method can be defined having order of convergence equal to 1.84. The derivative-free version of Halley’s method is comparable with the well-known Muller’s method, having identical order of convergence with that method. It is also possible to define a multipoint Halley Family. We will consider this in more generality in [15].

2 The order and asymptotic error of Halley Family.

We restrict ourselves to the problem of approximating real roots of functions defined on an interval.

Theorem 1.1. Assume that \( f(x) \) is three times continuously differentiable in an open interval containing a simple root \( \theta \). For each \( m \geq 3 \), there exists \( r > 0 \) such that given any \( x_0 \in N_r(\theta) = \{ x : |x - \theta| < r \} \), the fixed-point iteration

\[
x_{k+1} = H_m(x_k), \quad k = 1, 2, \ldots,
\]

is well-defined, it converges to \( \theta \) having order 3, satisfying

\[
\lim_{k \to \infty} \frac{(\theta - x_{k+1})}{(\theta - x_k)^3} = \begin{cases} 
-\frac{1}{6} \frac{f''''(\theta)}{f''(\theta)}, & \text{if } m > 3 \\
-\frac{1}{6} \frac{f''''(\theta)}{f''(\theta)} + \frac{3}{12} \frac{f'''(\theta)^2}{f''(\theta)^2}, & \text{if } m = 3.
\end{cases}
\]

Note that for \( m > 3 \), the asymptotic error constant is the same, it does not depend on the second derivative, and it is zero for the case where \( f(x) \) is a quadratic polynomial. In fact in this case the order of convergence of \( H_m \) is \( m \). This result follows from the \( m \)-th order convergence rate of \( B_m(x) \), see [11].

3
In order to prove Theorem 1.1 we first state and prove several auxiliary lemmas.

**Lemma 2.1.** Let $h_m(x) = \det(A_m(x))$. We have,

\[
\begin{align*}
  h_m &= f'h_{m-1} - \frac{1}{2}ff''h_{m-2}. & (i) \\
h'_m &= f''h_{m-1} + f'h'_{m-1} - \frac{1}{2}\left(f'f'' + ff''\right)h_{m-2} - \frac{1}{2}ff'h'_{m-2}. & (ii) \\
h''_m &= f''h_{m-1} + 2f'h'_{m-1} + f'^2h''_{m-1} - \frac{1}{2}\left((f'')^2 + 2f'f''' + f f^{(iv)}\right)h_{m-2} \\
&\quad - (f'f'' + ff''')h'_{m-2} - \frac{1}{2}ff''h'_{m-2}. & (iii)
\end{align*}
\]

**Proof.** We will only prove the first equation. The second and third equations are derived by straightforward differentiation. By expanding $h_m(x)$ along its first column we get,

\[
h_m(x) = f'(x)h_{m-1}(x) - f(x)det(\hat{A}_{m-1}(x)),
\]

where $\hat{A}_{m-1}(x)$ is the $(m-1) \times (m-1)$ matrix that replaces the first row of $A_{m-1}(x)$ by the vector $(f''(x)/2, 0, \ldots, 0)$. By expanding $det(\hat{A}_{m-1}(x))$ along its first row we get the desired formula. □.

**Lemma 2.2.** For all $m \geq 1$, we have

\[
\begin{align*}
  h_m(\theta) &= f'(\theta)^m. & (I) \\
h'_m(\theta) &= \frac{(m+1)}{2}f'(\theta)^{m-1}f''(\theta). & (II)
\end{align*}
\]

For $m = 1$, $h'_1(\theta) = f''(\theta)$, and for all $m > 1$, we have

\[
h''_m(\theta) = \frac{m(m+1)}{4}f'(\theta)^{m-2}f''(\theta)^2 + f'(\theta)^{m-1}f'''(\theta). & (III)
\]

**Proof.** The proof of (I) follows directly from the fact that $A_m(\theta)$ is upper triangular. Equivalently, it follows from the recursive equation implied by Lemma 2.1:

\[
h_m(\theta) = f'(\theta)h_{m-1}(\theta).
\]

To prove (II), from (ii) we get the recursive formula

\[
h'_m(\theta) = \frac{1}{2}f'(\theta)^{m-1}f''(\theta) + f'(\theta)h'_{m-1}(\theta).
\]

This implies that for each natural number $j \leq m - 1$, we have

\[
h'_m(\theta) = \frac{j}{2}f'(\theta)^{m-1}f''(\theta) + f'(\theta)^2h'_{m-j}(\theta).
\]
In particular, setting \( j = m - 1 \), and using that \( h'(\theta) = f''(\theta) \), the proof of (II) follows.

For \( m = 1 \), the proof of (III) is trivial. For \( m > 1 \), from (iii), (I), (II), and that \( f(\theta) = 0 \), we get the following recursive equation

\[
h''_m(\theta) = \frac{m}{2} f'(\theta)^{m-2} f''(\theta)^2 + f'(\theta) h''_{m-1}(\theta).
\]

Repeated application of the above recursion gives

\[
h''_m(\theta) = \frac{1}{2} f'(\theta)^{m-2} f''(\theta)^2 [m + (m - 1) + \cdots + 3] + f'(\theta)^{m-2} h''_2(\theta).
\]

It is easy to show that

\[
h''_2(\theta) = \frac{3}{2} f''(\theta) + f'(\theta) h''(\theta).
\]

Substituting the above into the previous equation and simplifying, we obtain the proof of (III).

\( \square \).

**Lemma 2.3.** For each \( m \geq 3 \), we have

\[
H'_m(\theta) = H''_m(\theta) = 0.
\]

\[
H'''_m(\theta) = \frac{f'''(\theta)}{f'(\theta)} + \frac{3}{2} \frac{f''(\theta)^2}{f'(\theta)^2}.
\]

For all \( m > 3 \), we have

\[
H'''_m(\theta) = \frac{f'''(\theta)}{f'(\theta)}.
\]

**Proof.** Let

\[
R_m(x) = \frac{h_{m-2}(x)}{h_{m-1}(x)}.
\]

Thus, \( H_m(x) = x - f(x) R(x) \). repeated differentiation gives

\[
H'_m(\theta) = 1 - (f'(\theta) R(\theta)).
\]

\[
H''_m(\theta) = -(f''(\theta) R(\theta) + 2 f'(\theta) R'(\theta)).
\]

\[
H'''_m(\theta) = -(f'''(\theta) R(\theta) + 3 f''(\theta) R'(\theta) + 3 f' R''(\theta)).
\]

We have

\[
R'_m = \frac{1}{h_{m-1}^2} \left( h'_{m-2} h_{m-1} - h_{m-2} h'_m \right).
\]

\[
R''_m = \frac{1}{h_{m-1}^2} \left( h''_{m-2} h_{m-1} - h_{m-2} h''_m \right) - 2 \frac{h'_{m-1}}{h_{m-1}} R'_m.
\]

From Lemma 2.2, we get

\[
R_m(\theta) = \frac{1}{f'(\theta)}.
\]
Also,
\[ R'_m(\theta) = \frac{1}{f'(\theta)^{2m-2}} \left( \frac{m-1}{2} f'(\theta)^{2m-4} f''(\theta) - \frac{m}{2} f'(\theta)^{2m-4} f''(\theta) \right) = \frac{1}{2} \frac{f''(\theta)}{f'(\theta)^2}. \]

From the same Lemma, for \( m > 3 \), we have
\[ R''_m(\theta) = \frac{1}{f'(\theta)^{2m-2}} \left( \frac{1}{4} [(m-2)(m-1) - (m-1)m] f'(\theta)^{2m-5} f''(\theta)^2 \right) + \frac{m f''(\theta)^2}{2 f'(\theta)^3}. \]
Thus,
\[ R''_m(\theta) = \frac{1}{2} \frac{f''(\theta)^2}{f'(\theta)^3}, \quad m > 3. \]

For \( m = 3 \), we get
\[ R''_3(\theta) = \frac{1}{f'(\theta)^3} \left( f''(\theta) f'(\theta)^2 - f'(\theta) \left( \frac{3}{2} f''(\theta)^2 + f'(\theta) f'''(\theta) \right) \right) + \frac{3 f''(\theta)^2}{2 f'(\theta)^3} = 0. \]

From the computed values of \( R_m(\theta) \), \( R'_m(\theta) \), and \( R''_m(\theta) \), the lemma follows. \( \square \)

Finally, to complete the proof of Theorem 1.1, we only need to apply Taylor’s theorem. Given that \( x_k \) is sufficiently close to the simple root \( \theta \), we have
\[ H_m(x_k) = \theta + H'_m(\theta)(x_k - \theta) + \frac{H''_m(\theta)}{2!} (x_k - \theta)^2 + \frac{H'''_m(\xi_k)}{3!} (x_k - \theta)^3, \]
where \( \xi_k \) lies between \( \theta \) and \( x_k \). This implies
\[ \frac{H_m(x_k) - \theta}{(x_k - \theta)^3} = \frac{H'''_m(\xi_k)}{3!}. \]
The above implies well-definedness of the fixed-point iteration, convergence, and gives the asymptotic error constant as \( H'''_m(\theta)/6 \), derived explicitly in Lemma 2.3. \( \square \)

References


