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NEWTON'S METHOD WITH MODIFIED FUNCTIONS

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Abstract. Applying the Newton method to a modified function

$$f(x)\,(x-\theta)^{\alpha} \qquad \text{where } \theta,\ \alpha \text{ are suitable parameters },$$

results in the iteration

$$x_{k+1} \;:=\; x_k - \frac{(x_k-\theta)\,f(x_k)}{(x_k-\theta)\,f'(x_k)+\alpha f(x_k)}\ ,$$

whose convergence is related to the convexity of f relative to the family of functions

$$\mathcal{F}_{\theta,\alpha} \;:=\; \left\{\frac{a+b\,(x-\theta)}{(x-\theta)^{\alpha}} \;:\; a,\,b\in\mathbb{R}\right\}$$

We study useful selections of the parameters α and θ, as well as the case where these are updated at each iteration.

1. Introduction

The **Newton method**

$$x_{k+1} \;:=\; x_k - \frac{f(x_k)}{f'(x_k)}\ , \quad k=0,1,2,\ldots \tag{1}$$

may perform better, near a zero ζ of f, if applied to a modified function $\widehat{f}$ with the same zero. Examples:

method	iteration	obtained by applying (1) to:
A 2nd order method for zeros with multiplicity m (known) [10, Chapter 8]	$x_{k+1} \;:=\; x_k - m\,\frac{f(x_k)}{f'(x_k)}$	$\widehat{f}(x) \;:=\; f^{1/m}(x)$
A 2nd order method for zeros of any multiplicity [15, Example 2–5]	$x_{k+1} \;:=\; x_k - \frac{f(x_k)}{f'(x_k) - \frac{f''(x_k)}{f'(x_k)}\,f(x_k)}$	$\widehat{f}(x) \;:=\; \frac{f(x)}{f'(x)}$
The **Halley** method: A 3rd order method ([1], [15], [13] and references therein)	$x_{k+1} \;:=\; x_k - \frac{f(x_k)}{f'(x_k) - \frac{f''(x_k)}{2f'(x_k)}\,f(x_k)}$	$\widehat{f}(x) \;:=\; \frac{f(x)}{\sqrt{f'(x)}}$

The above modified functions are special cases of

$$\widehat{f}(x) \;:=\; e^{-\int a(x)\,dx}\,f(x)\ ,\ \text{with a suitable integrand } a(x)\ , \tag{2}$$

for which the Newton method gives

$$x_{k+1} \;:=\; x_k - \frac{f(x_k)}{f'(x_k)-a(x_k)f(x_k)}\ , \quad k=0,1,2,\ldots \tag{3}$$

The order of (3) is determined by the first nonzero (continuous) derivative of its iteration function

$$\Phi_{(3)}(x) \;:=\; x - \frac{f(x)}{f'(x)-a(x)f(x)}$$

at the fixed point $\zeta=\Phi_{(3)}(\zeta)$, see e.g. [15, Theorem 2.2]. Differentiating $\Phi_{(3)}$ at ζ and substituting $f(\zeta)=0$ we get

$$\Phi'_{(3)}(\zeta) \;=\; 0\ , \quad \Phi''_{(3)}(\zeta) \;=\; \frac{f''(\zeta)-2\,a(\zeta)\,f'(\zeta)}{f'(\zeta)}\ ,$$

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showing that in general the order is 2 (as expected, since (3) is a Newton method). The order is 3 for the selection

$$a(x) \ := \ \frac{f''(x)}{2\,f'(x)} \tag{4}$$

which renders $\Phi''_{(3)}(\zeta) = 0$. Indeed, substituting (4) in (3) we get the Halley method

$$x_{k+1} \ := \ x_k - \frac{f(x_k)}{f'(x_k) - \dfrac{f''(x_k)}{2f'(x_k)}\, f(x_k)} \ , \quad k = 0, 1, 2, \ldots \tag{5}$$

Sometimes it is advantageous to modify f as a composition, (or transformation of variables),

$$\widehat{f}(x) \ := \ f(g(x)) \ , \quad \text{see e.g. [9]} \ ,$$

rather than the multiplicative form (2).

In this paper we consider a special case of (2)

$$\widehat{f}(x) \ := \ (x-\theta)^{\alpha}\, f(x) \ , \text{with suitable parameters } \theta \text{ and } \alpha \ , \tag{6}$$

corresponding to the selection of $a(x)$ as

$$a(x) \ := \ -\frac{\alpha}{x-\theta} \ . \tag{7}$$

Applying the Newton method to (6) (i.e. substituting (7) in (3)), we get

$$x_{k+1} \ := \ x_k - \frac{(x_k-\theta)\, f(x_k)}{(x_k-\theta)\, f'(x_k) + \alpha f(x_k)} \ , \quad k = 0, 1, 2, \ldots \tag{8}$$

The parameter θ may be adjusted in each iteration, in particular,

$$\theta_k \ := \ x_{k-1} \ , \quad \text{the last iterate,} \tag{9}$$

in which case (8) becomes

$$x_{k+1} \ := \ x_k - \frac{(x_k-x_{k-1})\, f(x_k)}{(x_k-x_{k-1})\, f'(x_k) + \alpha f(x_k)} \ , \quad k = 0, 1, 2, \ldots \tag{10}$$

A geometric interpretation of (8) is given in Theorem 1. First we require the following notation: two differentiable functions f and g are called **tangent** at a point x_k if $f(x_k) = g(x_k)$ and $f'(x_k) = g'(x_k)$, a fact denoted by $f \overset{x_k}{\approx} g$. Clearly

$$f(x) \overset{x_k}{\approx} g(x) \qquad \text{if and only if} \qquad (f(x)\, h(x)) \overset{x_k}{\approx} (g(x)\, h(x)) \tag{11}$$

whenever h is differentiable, and $h(x_k) \neq 0$.

Given θ and α, consider the function

$$F(x \,|\, \theta, \alpha) \ := \ \frac{a + b\,(x-\theta)}{(x-\theta)^{\alpha}} \tag{12}$$

which is tangent to f at x_k (the coefficients a and b are determined by the tangency $f(x) \overset{x_k}{\approx} F(x \,|\, \theta,\, \alpha)$). Note that $x = \theta$ is a zero of $F(x \,|\, \theta, \alpha)$ if $\alpha < 0$, and is a pole if $\alpha > 0$.

If $\theta \neq x_k$ it follows from (11) that

$$f(x) \overset{x_k}{\approx} \frac{a + b\,(x-\theta)}{(x-\theta)^{\alpha}} \qquad \text{if and only if} \qquad (x-\theta)^{\alpha}\, f(x) \overset{x_k}{\approx} a + b\,(x-\theta) \ . \tag{13}$$

The RHS of (13) states that the affine function

$$\ell(x) \ = \ a + b\,(x-\theta) \tag{14}$$

is tangent to $(x-\theta)^{\alpha}\, f(x)$ at x_k. Moreover, the function (12) and the affine function (14) have a common zero at

$$x \ = \ \theta - \frac{a}{b} \tag{15}$$

provided b is nonzero. We summarize:

Theorem 1. *Let f be differentiable, let θ, α be fixed, and let $x_k \neq \theta$ be a point where $(x_k - \theta)\, f'(x_k) + \alpha f(x_k) \neq 0$. The function*

$$F(x \,|\, \theta,\, \alpha) \;:=\; \frac{a + b\,(x-\theta)}{(x-\theta)^{\alpha}} \tag{12}$$

tangent to f at x_k has a zero at

$$x_{k+1} \;=\; x_k - \frac{(x_k-\theta)\, f(x_k)}{(x_k-\theta)\, f'(x_k) + \alpha f(x_k)} \tag{8}$$

which is the zero of the affine function

$$\ell(x) \;=\; a + b\,(x-\theta) \tag{14}$$

tangent at x_k to

$$\widehat{f}(x) \;:=\; (x-\theta)^{\alpha}\, f(x)\,. \tag{6}$$

Theorem 1 states that the iteration (8) is equivalent to finding the zero of the function (12) which is tangent to $f(x)$ at x_k .

The iterative method (8) uses the function (12) to interpolate f and f' at the single point x_k, thereby fixing the two free coefficients a and b (the parameters α and θ are fixed at the outset). In comparison, the rational interpolation methods (see e.g. [8], [7]) use a rational function, such as $(x-a)/\sum_{j=0}^{m} b_j\, x^j$ to interpolate f (or f and some of its derivatives) in as many points as needed to determine the coefficients. This was generalized to nonpolynomial interpolation in [2]. However, the iterative methods (8) and (10) are not covered by the theory in [8], [7] or [2], even if α is a positive integer (making (12) rational). In particular, the iterative method (10) uses information in an asymmetric way: f and f' at x_k, nothing at x_{k-1} (except x_{k-1} itself).

Outline of this paper:

Four "bad" examples, presenting situations where Newton method is inadequate, are given in § 2.

The iterative method (8) is related to a notion of generalized convexity discussed in § 3. Let $\mathcal{F}_{\theta,\alpha}$ be the family of functions (12), and let f be strictly $\mathcal{F}_{\theta,\alpha}$–convex. Then Theorem 2 shows the convergence of (8) to be monotone.

Useful selections of the parameters θ and α are indicated in § 4.

In § 5 we discuss the case where the parameters θ and α are updated in each iteration, in particular a quasi–Halley method (38) with order 2.41, using at each iteration the current values of f and f', and a previous (available) value of f'.

In § 6, the Newton and Halley steps, emanating from the same point, are compared in Theorem 4. Similarly, the Halley and quasi–Halley steps are compared in Theorem 5.

2. Bad examples for the Newton method

Examples 1–4 below illustrate what can go wrong with the Newton method. First we recall typical conditions for the convergence of (1), written as $x_{k+1} - x_k \;=\; -u_k$ where

(16) $$u_k \;:=\; \frac{f(x_k)}{f'(x_k)}\,, \quad k = 0, 1, 2, \ldots$$

is the k^{th} **Newton step**. Let x_0 be an initial point, and let J_0 be the interval with endpoints x_0 and $x_0 - 2\,u_0$, in which f is assumed twice–differentiable. The conditions

(17a) $$\sup_{x \in J_0} |f''(x)| \;=\; M$$

(17b) $$|f'(x_0)| \;\geq\; 2\,|u_0|\,M$$

are sufficient for the existence of a unique zero ζ of f in J_0, and for the convergence of (1) to that solution, see [10, Theorem 7.1]. If ζ is a simple root, the convergence is quadratic

(18) $$|x_{k+1} - \zeta| \;\leq\; \left|\frac{f''(\zeta)}{2\,f'(\zeta)}\right|\, |x_k - \zeta|^2\,.$$

Also, the conditions (17) hold throughout the iterations:

(19a) $$|f''(x_k)| \;\leq\; M$$

(19b) $$|f'(x_k)| \;\geq\; 2\,|u_k|\,M\,, \quad k = 1, 2, \ldots$$

Example 1 (Repulsion)**.** The function

(20) $$f_1(x) \;:=\; x^{1/3}$$

has a unique zero at 0. The Newton method diverges for any nonzero x_0: the iteration (1) gives $x_{k+1} = -2\,x_k$.

Example 2 (Linear convergence for multiple zeros)**.** The function

$$f_2(x) := x^p$$

has a multiple zero at 0 if $p \geq 2$. The Newton method gives $x_{k+1} = \frac{p-1}{p}\,x_k$, i.e. linear convergence. For $p = 2$, the conditions (17) hold at all x_0, but convergence is linear since the root $\zeta = 0$ is multiple.

Example 3 (Large step)**.** Let

$$f_3(x) := e^{1-x} - 1 \tag{21}$$

If $x_0 = 1 + \ln\,a$ where $a > 0$ is large, then the first step $u_0 = -(a-1)$ is large and negative, as is $x_1 = \ln\,a - a$. Many consecutive steps are ≈ 1. For example,

$$x_0 = 10,\ x_1 = -8092.08,\ x_2 = -8091.08,\ x_3 = -8090.08, \ldots$$

and thousands of iterations are required to approach the root $\zeta = 1$.

Example 4 (Wrong direction)**.** The function

$$f_4(x) := x\,e^{-x} \tag{22}$$

has a unique zero at 0. The derivative of f_4 is zero for $x = 1$, and negative for $x > 1$. For any initial $x_0 > 1$ the Newton iterates move away from the zero. For example: $x_0 = 2,\ x_1 = 4,\ x_2 = 5.3333,\ x_3 = 6.5641,\ x_4 = 7.74382, \ldots$

3. Convexity and monotone convergence

The iterative method (8) is related to a notion of generalized convexity discussed below.

All functions in this section are twice continuously differentiable in a real interval I. The function f is **supported** by g at x_0 if

$$f(x_0) = g(x_0) \quad \text{and} \quad f(x) \geq g(x) \quad \text{for all } x \in I\ ,$$

and **supported strictly** if the above inequality is strict for all $x \neq x_0$.

Let $\mathcal{F}$ be a family of functions $: I \to \mathbb{R}$. The function f is called [**strictly**] $\mathcal{F}$**–convex** if at each point in I it is [strictly] supported by a member of $\mathcal{F}$, see [3], [4].

We use the family of functions (12)

$$\mathcal{F}_{\theta,\alpha} := \left\{ \frac{a + b\,(x-\theta)}{(x-\theta)^\alpha} \ :\ a,\, b \in \mathbb{R} \right\} \tag{23}$$

where θ and α are given parameters. In particular, for $\alpha = 0$ and any θ, the **affine functions**

$$\mathcal{F}_{\theta,0} := \{a + b\,(x-\theta)\ :\ a,\, b \in \mathbb{R}\}\ . \tag{24}$$

Since convex functions are supported by affine functions, $\mathcal{F}_{\theta,0}$–convexity is the same as ordinary convexity.

Lemma 1. *Let I be a real interval, let $f : I \to \mathbb{R}$ be a finite function, and let $\theta, \alpha \in \mathbb{R}$ be given, with $\theta \notin I$. If* $\left\{ \begin{array}{l} (x-\theta)^\alpha > 0 \\ (x-\theta)^\alpha < 0 \end{array} \right.$ $\forall x \in I$, *then f is $\mathcal{F}_{\theta,\alpha}$–convex in I if and only if $(x-\theta)^\alpha\,f(x)$ is* $\left\{ \begin{array}{l} \textit{convex} \\ \textit{concave} \end{array} \right.$ *in I.*

Proof. Let $\mathcal{F}$ be a family of functions $: I \to \mathbb{R}$, and p a function positive in I. Then for any function $f : I \to \mathbb{R}$,

$$f \text{ is } \mathcal{F}\text{–convex if and only if the product function } (p\,f) \text{ is } (p\,\mathcal{F})\text{–convex}$$

where $(p\,\mathcal{F})$ is the family $\{p\,F\ :\ F \in \mathcal{F}\}$. The lemma is then proved by the observations:
(a) $\mathcal{F}_{\theta,0} = (x-\theta)^\alpha\,\mathcal{F}_{\theta,\alpha}$,
(b) $\mathcal{F}_{\theta,0}$–convexity is ordinary convexity, and
(c) f is convex iff $-f$ is concave. □

In Lemma 1 the point θ is assumed outside the interval I, so that

$$(x-\theta)^\alpha \neq 0\ , \quad \forall x \in I\ . \tag{25}$$

If θ is updated at each iteration, according to (9), we update I accordingly by deleting the interval between θ and x_k, to assure that (25) holds throughout the iterations.

Lemma 1 can be explained using the 2nd derivative characterization of convexity. The family (23) satisfies the 2nd order differential equation

$$y'' \; = \; -\frac{2\,\alpha}{x-\theta}\,y' - \frac{\alpha\,(\alpha-1)}{(x-\theta)^2}\,y \; . \tag{26}$$

It follows from [11] and [3] that the $\mathcal{F}_{\theta,\alpha}$–convexity of f is characterized by the corresponding 2nd order differential inequality

$$f''(x) \; \geq \; -\frac{2\,\alpha}{x-\theta}\,f'(x) - \frac{\alpha\,(\alpha-1)}{(x-\theta)^2}\,f(x) \; . \tag{27}$$

Consider the 2nd derivative of the modified function $\widehat{f}(x) := (x-\theta)^{\alpha} f(x)$

$$\widehat{f}''(x) \; = \; (x-\theta)^{\alpha}\,f''(x) + 2\,\alpha\,(x-\theta)^{\alpha-1}\,f'(x) + \alpha\,(\alpha-1)\,(x-\theta)^{\alpha-2}\,f(x) \; .$$

If $(x-\theta)^{\alpha} > 0$ holds in I then $\widehat{f}'' \geq 0$ ($\widehat{f}$ is convex) iff the inequality (27) holds, i.e. f is $\mathcal{F}_{\theta,\alpha}$–convex. Similarly, if $(x-\theta)^{\alpha} < 0$ in I then (27) is equivalent to $\widehat{f}'' \leq 0$.

Convexity is related to the monotone convergence of Newton's iterations

$$x_{k+1} \; := \; x_k - \frac{f(x_k)}{f'(x_k)} \; , \quad k = 0,1,2,\ldots \tag{1}$$

If f is strictly convex and $f(x_k) > 0$ then $f(x_j) > 0$ for all $j > k$, i.e. f is positive at all successive points. If $f(x_0) < 0$ then $f(x_1) > 0$ and thereafter f is positive at all iterations. An analogous result holds for the iteration (8).

Theorem 2. *Let f be strictly $\mathcal{F}_{\theta,\alpha}$–convex in an interval I, $\theta \notin I$, and let I include x_0 and all iterates generated by*

$$x_{k+1} \; = \; x_k - \frac{(x_k-\theta)\,f(x_k)}{(x_k-\theta)\,f'(x_k) + \alpha f(x_k)} \; , \quad k = 0,1,2,\ldots \tag{8}$$

(a) If $f(x_0) > 0$ then f is positive for all successive points generated by (8).
(b) If $f(x_0) < 0$ then $f(x_1) > 0$ and thereafter f is positive at all iterations.

Proof. Follows from Theorem 1 which shows that (8) is equivalent to the Newton method applied to the modified function $(x-\theta)^{\alpha}\,f(x)$, and Lemma 1. □

For other applications of generalized convexity in Newton's method see [4, § 9], [5].

4. The method (8) with constant α

Consider the selection of the parameter α in (8) or (10). If monotone convergence is desired, the key to the selection is provided by the inequality (27).

For example, consider the case $x > \theta$ and $\alpha \leq 1$. If $f(x) > 0$ and $f'(x) > 0$ it follows that the RHS of (27) has the same sign as α. Therefore, if the second derivative f'' is bounded, there is an $\alpha < 0$ satisfying (27). A positive α makes sense, in this case, only if $f'' > 0$, i.e. if f is strictly convex.

In §§ 4.1–4.2 we consider the special cases $\alpha = -1$ [$\alpha = 1$] as representative of negative [positive] α.

4.1. $\alpha = -1$**.** Here the family (23) consists of the quadratic functions with a zero at θ,

$$\mathcal{F}_{\theta,-1} \; = \; \{a\,(x-\theta) + b\,(x-\theta)^2 \; : \; a,\, b \in \mathbb{R}\} \; . \tag{28}$$

A function $F \in \mathcal{F}_{\theta,-1}$ supporting f at x_k has its second zero at

$$x_{k+1} \; = \; x_k - \frac{(x_k-\theta)\,f(x_k)}{(x_k-\theta)\,f'(x_k) - f(x_k)} \; , \tag{29}$$

which is (8) with $\alpha = -1$. The modified function $\widehat{f}$ of (6) is

$$\widehat{f}(x) \; = \; \frac{f(x)}{x-\theta} \tag{30}$$

its pole at θ acts as a barrier, repulsing the iterates of (8).

The method (29) becomes, for the selection (9),

$$x_{k+1} \; = \; x_k - \frac{(x_k-x_{k-1})\,f(x_k)}{(x_k-x_{k-1})\,f'(x_k) - f(x_k)} \; , \quad k = 0,1,2,\ldots \tag{31}$$

requiring two initial points x_0 and x_{-1}. Since x_{-1} is the initial barrier, the initial point x_0 should be between the sought zero ζ and x_{-1}. Thus to apply (31) it is required to know on which side of x_0 lies ζ.

As long as the barrier is "away" from the sought zero, the step length $|x_{k+1} - x_k|$ of (31) is shorter than a corresponding step length of the Newton method (1).

Example 5. We apply the method (31) to the function

$$f_1(x) := x^{1/3} \tag{20}$$

of Example 1. The table below gives a selected iterate x_k for various combinations of x_0 and x_{-1}.

x_{-1}	x_0	iterate
1.01	1	$x_{10} = 0.901845$
		$x_{100} = 0.193404$
1.1	1	$x_{20} = -2.31673\ 10^{-6}$
1.2	1	$x_{10} = -1.13652\ 10^{5}$
1.5	1	$x_3 = 0$

The table shows tricky dependence on x_{-1}. One expects short steps and slow convergence if x_{-1} is very close to x_0. In general, reducing $|x_{-1} - x_0|$ does not retain convergence, as shown by the last two entries in the table.

Example 6. We apply the method (31) to the function

$$f_3(x) := e^{1-x} - 1 \tag{21}$$

of Example 3. In contrast with the Newton method, the method (31) converges fast for all $1 < x_0$, as long as the initial barrier x_{-1} is to the right of x_0. Examples:

x_{-1}	x_0	x_1	x_2	x_3	x_4	x_5
20	10	0.0123266	0.681959	0.875605	0.948526	0.978248
6	4	2.1897	1.17941	1.01489	1.00114	1.00008

Example 7. We apply the method (31) to the function

$$f_4(x) := x\,e^{-x} \tag{22}$$

of Example 4. The table below gives a selected iterate x_k for various combinations of x_0 and x_{-1}.

x_{-1}	x_0	iterate
2.1	2	$x_{10} = 0.733696$
		$x_{100} = 2.25589\ 10^{-15}$
2.5	2	$x_7 = 9.93368\ 10^{-7}$
3	2	$x_2 = 0$
3.5	2	$x_5 = -2.20516$
		$x_{300} = -0.0473647$

Example 8. ([6, p. 178, Example 4]) We use (31) to find a root of

$$f(x) := e^{-x} - \sin x$$

x_{-1}	x_0	x_1	x_2	x_3	x_4	x_5
0.5	0.6	0.586979	0.588741	0.588504	0.588536	0.588532

This is the smallest root. There are infinitely many roots lying close to π, 2π, 3π, ... which can be computed recursively by (31) if the initial barrier x_{-1} is taken between the initial x_0 and the last found root. For example, to compute the root near 2π we can use (31) with $x_{-1} = 4$ and $x_0 = 5$,

x_{-1}	x_0	x_1	x_2	x_3	x_4	x_5
4	5	5.76880	6.09502	6.21599	6.25999	6.27596

In contrast, for the same initial $x_0 = 5$ the Newton method converges to the root closest to 3π,

x_0	x_1	x_2	x_3	x_4	x_5
5	8.32528	10.2880	9.11860	9.43463	9.42469

i.e. the nearest root 6.27596 is skipped.

4.2. $\alpha = 1$. In this case the family $\mathcal{F}_{\theta,\alpha}$ of (23) consists of the hyperbolas with pole in θ

$$\mathcal{F}_{\theta,1} = \left\{ \frac{a}{x-\theta} + b \,:\, a, b \in \mathbb{R} \right\} . \tag{32}$$

The parameter θ should be sufficiently far from x_k, for stability reasons. For $\alpha = 1$ the method (8) gives

$$x_{k+1} = x_k - \frac{(x_k - \theta)\, f(x_k)}{(x_k - \theta)\, f'(x_k) + f(x_k)} , \quad k = 0, 1, 2, \ldots \tag{33}$$

and the inequality (27) becomes,

$$f''(x) \geq -\frac{2}{x-\theta}\, f'(x) .$$

For $x < \theta$ it follows that $\alpha = 1$ is a good choice if f is strictly convex and $|f'|$ is sufficiently small, for example, near a multiple root.

5. The quasi–Halley method

In this section we consider a version of (10), where also α is updated at each iteration.

The derivatives of the iteration function of (8)

$$\Phi_{(8)}(x) \ := \ x - \frac{(x-\theta)\, f(x)}{(x-\theta)\, f'(x) + \alpha\, f(x)} \tag{34}$$

at a fixed point $\zeta \neq \theta$, where necessarily $f(\zeta) = 0$, are

$$\Phi'_{(8)}(\zeta) \ = \ 0\,, \tag{35a}$$

$$\Phi''_{(8)}(\zeta) \ = \ \frac{2\,\alpha\, f'(\zeta) + (\zeta-\theta)\, f''(\zeta)}{(\zeta-\theta)\, f'(\zeta)}\,. \tag{35b}$$

The parameter α may be chosen so as to make $|\Phi''_{(8)}(\zeta)|$ in (35b) as small as possible. The ideal choice (making $|\Phi''_{(8)}(\zeta)| = 0$) is

$$\alpha \ = \ -\frac{(\zeta-\theta)\, f''(\zeta)}{2\, f'(\zeta)} \tag{36}$$

If f'' is continuous and θ is close to ζ, then (36) can be approximated as

$$\alpha \ \approx \ -\frac{f'(\zeta) - f'(\theta)}{2\, f'(\zeta)}$$

which can be implemented, using (9) for θ, by the selection

$$\alpha_k \ := \ -\frac{f'(x_k) - f'(x_{k-1})}{2\, f'(x_k)}\,. \tag{37}$$

Substituting (9) and (37) in (8) gives the **quasi–Halley method**

$$x_{k+1} \ := \ x_k - \frac{f(x_k)}{f'(x_k) - \dfrac{f'(x_k) - f'(x_{k-1})}{2\,(x_k - x_{k-1})\, f'(x_k)}\, f(x_k)}\,, \quad k = 0, 1, 2, \ldots \tag{38}$$

The first iteration uses x_0 and an additional point x_{-1} . Alternatively, the quasi–Halley method (38) can be obtained from (3) by approximating (4) at x_k as

$$a(x_k) \ = \ \frac{f''(x_k)}{2\, f'(x_k)} \ \approx \ \frac{f'(x_k) - f'(x_{k-1})}{2\,(x_k - x_{k-1})\, f'(x_k)}\,.$$

The quasi–Halley method requires only the current values of f and f', and a previous (available) value of f', while the Halley method uses the current f, f' and f''. The order of the quasi–Halley method is ≥ 2.41 (see Theorem 3), as compared with order 3 for the Halley method.

The quasi–Halley method (38) is expected to perform, on the average, worse than the Halley method (5). Indeed, for $f(x) = x^{1/3}$ the table below shows convergence of (5) and divergence of (38). However, the two methods perform similarly for the other examples in the table, and in general for sufficiently smooth functions. In particular, both methods diverge for $x\, e^{-x}$ and $x_0 \geq 2$.

This similarity is explained in Theorem 5 which gives a local comparison of the Halley method and the quasi–Halley method.

function	method	initial point(s)	x_1	x_2	x_3	x_4	x_5
$x^{1/3}$	Halley	$x_0 = 1$	-0.5	0.25	-0.125	0.0625	-0.0312
	quasi–Halley	$x_{-1} = 1.1,\, x_0 = 1$	-0.559693	1.4699	-0.755481	2.01688	-0.995203
$x\, e^{-x}$	Halley	$x_0 = 2$	4	6.4	8.69177	10.9142	13.0937
	quasi–Halley	$x_{-1} = 2.1,\, x_0 = 2$	4.09816	6.82057	4.60104	6.27622	25.7395
$x^3 - 10$	Halley	$x_0 = 2$	2.15384	2.15443	2.15443	2.15443	2.15443
	quasi–Halley	$x_{-1} = 2.5,\, x_0 = 2$	2.15238	2.15443	2.15443	2.15443	2.15443
$e^{1-x} - 1$	Halley	$x_0 = 10$	8.00049	6.00413	4.03079	2.21501	1.00018
	quasi–Halley	$x_{-1} = 11,\, x_0 = 10$	6.83728	0.357585	0.849529	1	1
$x^4 + 2x^2$	Halley	$x_0 = 1$	0.4	0.135137	0.045055	0.015018	0.005006
	quasi–Halley	$x_{-1} = 1.1,\, x_0 = 1$	0.370739	0.009415	0.002829	0.000943	0.000314

The quasi–Halley method is usually better than the Halley method in the case of multiple roots (see e.g. the last example in the above table). Indeed, the quasi–Halley method "remembers" the last iterate, and is therefore less sensitive to the multiplicity of the root.

We illustrate next the Halley and quasi–Halley methods for complex roots.

Example 9. ([6, p. 177, Example 3]) Consider the complex polynomial

$$f(z) \;:=\; z^5 + (7-2\,i)\,z^4 + (20-12\,i)\,z^3 + (20-28\,i)\,z^2 + (19-12\,i)\,z + (13-26\,i)$$

One of the five roots is found by the Halley and quasi–Halley methods as follows.

iterate	Halley method $x_0 = 3\,i$	quasi–Halley method $x_{-1} = 1,\, x_0 = 3\,i$
x_1	$-0.499312 + 2.19129\,i$	$-0.343620 + 2.52897\,i$
x_2	$-0.987763 + 1.89479\,i$	$-1.01552 + 1.84006\,i$
x_3	$-1.00026 + 1.99934\,i$	$-1.02212 + 1.97408\,i$
x_4	$-1 + 2\,i$	$-0.999892 + 2\,i$
x_5		$-1 + 2\,i$

For simple roots of sufficiently smooth functions, the order of convergence of the quasi–Halley method is 2.41:

Theorem 3. *If f'' is Lipschitz continuous near a root ζ , if $f'(\zeta) \neq 0$, and if the iterates* (38) *converge to ζ, then as $k \to \infty$,*

$$|x_{k+1} - \zeta| \;=\; O\left(|x_k - \zeta|^{1+\sqrt{2}}\right) \tag{39}$$

Proof. The iteration function of (38) at x_k is

$$\Phi_{(38)}(x) \;=\; x - \frac{f(x)}{f'(x) - \left(\dfrac{f'(x) - f'(x_{k-1})}{2(x - x_{k-1})f'(x)}\right) f(x)}$$

and its second derivative at the zero ζ is

$$\Phi''_{(38)}(\zeta) \;=\; \frac{f''(\zeta)}{f'(\zeta)} - \frac{f'(\zeta) - f'(x_{k-1})}{(\zeta - x_{k-1})f'(\zeta)} \;=\; \frac{f''(\zeta) - f''(\xi)}{f'(\zeta)}$$

for some ξ between x_{k-1} and ζ. Since f'' is Lipschitz continuous

$$\begin{aligned} |f''(\zeta) - f''(\xi)| \;&\leq\; L\,|\zeta - \xi|\;, \quad \text{for some } L\,. \\ \therefore\;\; |\Phi''_{(38)}(\zeta)| \;&\leq\; \frac{L\,|\zeta - \xi|}{|f'(\zeta)|} \;\leq\; \frac{L\,|x_{k-1} - \zeta|}{|f'(\zeta)|}\,. \\ \therefore\;\; |x_{k+1} - \zeta| \;&\approx\; \frac{|\Phi''_{(38)}(\zeta)|}{2}\,|x_k - \zeta|^2 \;\approx\; \frac{L}{2\,|f'(\zeta)|}\,|x_{k-1} - \zeta|\,|x_k - \zeta|^2\,. \\ \therefore\;\; |x_{k+1} - \zeta| \;&=\; O\left(|x_{k-1} - \zeta|^{\gamma^2}\right) \;=\; O\left(|x_{k-1} - \zeta|^{2\gamma+1}\right)\;, \end{aligned} \tag{40}$$

where the order of convergence, γ, satisfies the quadratic equation

$$\gamma^2 - 2\gamma - 1 = 0\,.$$

□

Other first–derivative methods, with order $1+\sqrt{2}$, are known, see e.g. Method 9a in [15, p. 234]. Since the second inequality in (40) is strict, the quasi-Halley method may in fact have a higher order, i.e. its order γ satisfies

$$1 + \sqrt{2} \;\leq\; \gamma \;<\; 3\,. \tag{41}$$

The possibility that $1+\sqrt{2} < \gamma$ is supported by numerical experience, and the results of the next section, showing that (for sufficiently smooth functions) the quasi-Halley method is virtually indistinguishable from the Halley method, near a root to which both converge.

6. Comparison of steps

Iterative methods can be compared locally by comparing their steps at given points. The steps can be compared in terms of **length**, as we do here, or by their effect on the function value, see [2].

The proofs in this section are tedious, hence omitted.

We first compare the steps of the Newton and Halley methods, assuming both steps emanate from the same point x_k, arrived at by Newton's method. This corresponds to a hypothetical situation where at an iterate x_k of Newton's method we have an option of continuing (and making a Newton step) or switching to the Halley method (5), making a **Halley step**

$$h_k \;:=\; \frac{f(x_k)}{f'(x_k) - \dfrac{f''(x_k)}{2f'(x_k)}\,f(x_k)} \;, \quad k = 0, 1, 2, \ldots \tag{42}$$

To simplify the writing we denote by f_k the function f evaluated at x_k . Similarly, f_k' and f_k'' denote the derivatives f' , f'' evaluated at x_k . The steps to be compared are

$$u_k \;:=\; \frac{f_k}{f_k'} \quad \text{and} \quad h_k \;:=\; \frac{f_k}{f_k' - \dfrac{f_k''}{2f_k'}\,f_k} \;.$$

The next lemma gives a condition for the Newton step u_k and the Halley step h_k to have the same sign.

Lemma 2. *The steps u_k and h_k have the same sign iff*

$$|f_k'|^2 \;>\; \frac{f_k''\,f_k}{2} \;, \tag{43}$$

in which case

$$|h_k| \;\geq\; |u_k| \quad \text{if} \quad f_k f_k'' \;\geq\; 0 \;,$$
$$|h_k| \;<\; |u_k| \quad \text{if} \quad f_k f_k'' \;<\; 0 \;.$$

It is reasonable to assume that conditions (19) hold at the point x_k, which is arrived at by the Newton method, and where the steps u_k and h_k are compared. Under these conditions, we have the following comparison of the Newton and Halley steps.

Theorem 4. *If conditions* (19) *hold, then the Newton step u_k and the Halley step h_k have the same sign, and are related by*

$$\frac{2}{3}\,|u_k| \;\leq\; |h_k| \;\leq\; \frac{4}{3}\,|u_k| \;. \tag{44}$$

We next compare the Halley step h_k of (42) and the quasi–Halley step

$$q_k \;:=\; \frac{f(x_k)}{f'(x_k) - \dfrac{f'(x_k) - f'(x_{k-1})}{2\,(x_k - x_{k-1})\,f'(x_k)}\,f(x_k)} \;, \quad k = 0, 1, 2, \ldots \tag{45}$$

evaluated at the same point x_k arrived at by the Newton method.

Theorem 5. *Let f have continuous third derivative in the interval J_0, and let*

$$\sup_{x \in J_0} |f'''(x)| \;=\; N \;.$$

If conditions (19) *hold, then the Halley step h_k and the quasi–Halley step q_k are related by*

$$|h_k - q_k| \;\leq\; \frac{N}{2\,|f_k'|}\,|u_{k-1}|^3 \;. \tag{46}$$

Theorem 5 gives a comparison of the Halley step h_k and the quasi–Halley step q_k in terms of the underlying Newton step. If the point x_k is sufficiently close to a root, so that the last Newton step u_{k-1} is small, then the steps h_k and q_k are close within $O(|u_{k-1}|^3)$.

If the two steps h_k and q_k are compared at a point x_k arrived at by the Halley method, we can show that

$$|h_k - q_k| \;=\; O(|h_{k-1}|^3) \;,$$

as can be expected from Theorem 5 and the comparison between the Newton and Halley steps in Theorem 4.

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References

[1] G. Alefeld, *On the convergence of Halley's method*, Amer. Math. Monthly **88**(1981), 530–536.
[2] J. Barzilai and A. Ben-Tal, *Nonpolynomial and inverse interpolation for line search: Synthesis and convergence rates*, SIAM J. Numer. Anal. **19**(1982), 1263–1277.
[3] A. Ben-Tal and A. Ben-Israel, *A generalization of convex functions via support properties*, J. Austral. Math. Soc. **21A**(1976), 341–361.
[4] A. Ben-Tal and A. Ben-Israel, *$\mathcal{F}$–convex functions: Properties and applications*, pp. 301–334 in [14]
[5] S.L. Brumelle and M.L. Puterman, *Newton's method for W–convex operators*, pp. 399–414 in [14]
[6] C.-E. Fröberg, *Numerical Mathematics: Theory and Computer Applications*, The Benjamin/Cummings Publishing Co., 1985
[7] P. Jarratt, *A rational iteration function for solving equations*, Computer J. **9**(1966), 304–307.
[8] P. Jarratt and D. Nudds, *The use of rational functions in the iterative solution of equations on a digital computer*, Computer J. **8**(1965), 62–65.
[9] A. Melman, *Numerical solution of a secular equation*, Numer. Math. **69**(1995), 483–493.
[10] A.M. Ostrowski, *Solution of Equations in Euclidean and Banach Spaces*, 3rd Edition, Academic Press, 1973
[11] M.M. Peixoto, *Generalized convex functions and second order differential inequalities*, Bull. Amer. Math. Soc. **55**(1949), 563–572.
[12] A. Rich, J. Rich and D. Stoutemyer, DERIVE *User Manual*, Soft Warehouse, Inc., 3660 Waialae Avenue, Suite 304, Honolulu, Hawaii, 96816-3236.
[13] T.R. Scavo and J.B. Thoo, *On the geometry of Halley's method*, Amer. Math. Monthly **102**(1995), 417–426.
[14] S. Schaible and W.T. Ziemba (editors), *Generalized Concavity in Optimization and Economics*, Academic Press, 1981
[15] J.F. Traub, *Iterative Methods for the Solution of Equations*, Prentice–Hall, 1964

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