NEWTON’S METHOD WITH MODIFIED FUNCTIONS

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ABSTRACT. Applying the Newton method to a modified function
\[ f(x) = (x - \theta)^\alpha \]
where \( \theta, \alpha \) are suitable parameters, results in the iteration
\[ x_{k+1} := x_k - \frac{f(x_k)}{f'(x_k)} \]
whose convergence is related to the convexity of \( f \) relative to the family of functions
\[ F_{\theta, \alpha} := \{ a + b(x - \theta):(x - \theta)^\alpha : a, b \in \mathbb{R} \} \]
We study useful selections of the parameters \( \alpha \) and \( \theta \), as well as the case where these are updated at each iteration.

1. Introduction

The Newton method
\[ x_{k+1} := x_k - \frac{f(x_k)}{f'(x_k)} , \quad k = 0, 1, 2, \ldots \]
may perform better, near a zero \( \zeta \) of \( f \), if applied to a modified function \( \hat{f} \) with the same zero. Examples:

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

The above modified functions are special cases of
\[ \hat{f}(x) := e^{-\int a(x) \, dx} f(x) , \quad \text{with a suitable integrand} \ a(x) , \]
for which the Newton method gives
\[ x_{k+1} := x_k - \frac{f(x_k)}{f'(x_k) - a(x_k)f(x_k)} , \quad k = 0, 1, 2, \ldots \]
The order of (3) is determined by the first nonzero (continuous) derivative of its iteration function
\[ \Phi_{\zeta}(x) := x - \frac{f(x)}{f'(x) - a(x)f(x)} \]
at the fixed point \( \zeta = \Phi_{\zeta}(\zeta) \), see e.g. [15, Theorem 2.2]. Differentiating \( \Phi_{\zeta} \) at \( \zeta \) and substituting \( f(\zeta) = 0 \) we get
\[ \Phi'_{\zeta}(\zeta) = 0 , \quad \Phi''_{\zeta}(\zeta) = \frac{f''(\zeta) - 2a(\zeta) f'(\zeta)}{f'(\zeta)} , \]

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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

\[ a(x) := \frac{f''(x)}{2f'(x)} \]

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

\[ x_{k+1} := x_k - \frac{f(x_k)}{f'(x_k)} \left( f(x_k) - \frac{f''(x_k)}{2f'(x_k)} f(x_k) \right), \quad k = 0, 1, 2, \ldots \]

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

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

rather than the multiplicative form (2).

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

\[ \tilde{f}(x) := (x - \theta)^\alpha f(x), \]

with suitable parameters \( \theta \) and \( \alpha \), corresponding to the selection of \( a(x) \) as

\[ a(x) := -\frac{\alpha}{x - \theta}. \]

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

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

The parameter \( \theta \) may be adjusted in each iteration, in particular,

\[ \theta_k := x_{k-1}, \quad \text{the last iterate,} \]

in which case (8) becomes

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

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

\[ f(x) \preceq g(x) \quad \text{if and only if} \quad (f(x) h(x)) \preceq (g(x) h(x)) \]

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

Given \( \theta \) and \( \alpha \), consider the function

\[ F(x|\theta, \alpha) := \frac{a + b(x - \theta)}{(x - \theta)^\alpha}, \]

which is tangent to \( f \) at \( x_k \) (the coefficients \( a \) and \( b \) are determined by the tangency \( f(x) \preceq F(x|\theta, \alpha) \)). 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

\[ f(x) \preceq \frac{a + b(x - \theta)}{(x - \theta)^\alpha} \quad \text{if and only if} \quad (x - \theta)^\alpha f(x) \preceq a + b(x - \theta). \]

The RHS of (13) states that the affine function

\[ \ell(x) = a + b(x - \theta) \]

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

\[ x = \theta - \frac{a}{b} \]

provided \( b \) is nonzero. We summarize:
Let $f$ be differentiable, let $\theta$, $\alpha$ 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

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

(12)

tangent to $f$ at $x_k$ has a zero at

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

(8)

which is the zero of the affine function

$$ \ell(x) = a + b(x - \theta) $$

(14)

tangent at $x_k$ to

$$ \hat{f}(x) := (x - \theta)^\alpha f(x) $$

(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 $\alpha$ and $\theta$ are fixed at the outset). In comparison, the rational interpolation methods (see e.g. [8], [7]) use a rational function, such as $(x - a)/\sum b_j x^j$ 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 $\alpha$ 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 $F_{\theta, \alpha}$ be the family of functions (12), and let $f$ be strictly $F_{\theta, \alpha}$–convex. Then Theorem 2 shows the convergence of (8) to be monotone.

In § 5 we discuss the case where the parameters $\theta$ and $\alpha$ 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

$$ u_k := \frac{f(x_k)}{f'(x_k)} $$

(16)

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

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

(17a)

$$ |f'(x_0)| \geq 2 |u_0| M $$

(17b)

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

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

(18)

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

$$ |f''(x_k)| \leq M $$

(19a)

$$ |f'(x_k)| \geq 2 |u_k| M $$

(19b)

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

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

(20)
has a unique zero at 0. The Newton method diverges for any nonzero \( x_0 \): the iteration (1) gives \( x_{k+1} = -2x_k \).

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

\[
f_2(x) := x^p
\]

has a multiple zero at 0 if \( p > 2 \). 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

\[
f_3(x) := e^{1-x} - 1
\]

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 \( \approx 1 \). 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

\[
f_4(x) := x e^{-x}
\]

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

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

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

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

We use the family of functions (12)

\[
F_{\theta, \alpha} := \{ a + b(x - \theta) \over (x - \theta)^\alpha : a, b \in \mathbb{R} \}
\]

where \( \theta \) and \( \alpha \) are given parameters. In particular, for \( \alpha = 0 \) and any \( \theta \), the affine functions

\[
F_{\theta, 0} := \{ a + b(x - \theta) : a, b \in \mathbb{R} \}.
\]

Since convex functions are supported by affine functions, \( F_{\theta, \alpha} \)-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

\[
\begin{cases}
(x - \theta)^\alpha > 0 & \forall x \in I, \\
(x - \theta)^\alpha < 0 & \forall x \in I.
\end{cases}
\]

Then \( f \) is \( F_{\theta, \alpha} \)-convex in \( I \) if and only if \( (x - \theta)^\alpha f(x) \) is \( \{ \text{convex} \} \) in \( I \).

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

\[
f \text{ is } F \text{-convex if and only if the product function } (p f) \text{ is } (p F) \text{-convex}
\]

where \( (p F) \) is the family \( \{ pF : F \in F \} \). The lemma is then proved by the observations:

(a) \( F_{\theta, 0} = (x - \theta)^\alpha F_{\theta, \alpha} \),

(b) \( F_{\theta, 0} \)-convexity is ordinary convexity, and

(c) \( f \) is convex iff \( -f \) is concave. \( \square \)

In Lemma 1 the point \( \theta \) is assumed outside the interval \( I \), so that

\[
(x - \theta)^\alpha \neq 0, \quad \forall x \in I.
\]

If \( \theta \) is updated at each iteration, according to (9), we update \( I \) accordingly by deleting the interval between \( \theta \) 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

\begin{equation}
\frac{d^2y}{dx^2} = -\frac{2\alpha}{x-\theta} \frac{dy}{dx} - \frac{\alpha(\alpha-1)}{(x-\theta)^2} y.
\end{equation}

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

\begin{equation}
f''(x) \geq -\frac{2\alpha}{x-\theta} f'(x) - \frac{\alpha(\alpha-1)}{(x-\theta)^2} f(x).
\end{equation}

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

\[ \hat{f}''(x) = (x-\theta)^{\alpha-2} f''(x) + 2\alpha (x-\theta)^{\alpha-1} f'(x) + \alpha(\alpha-1)(x-\theta)^{\alpha-2} f(x). \]

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

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

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

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 $F_{\theta,\alpha}$-convex in an interval $I$, $\theta \notin I$, and let $I$ include $x_0$ and all iterates generated by

\[ x_{k+1} = x_k - \frac{(x_k-\theta) f(x_k)}{f'(x_k) + \alpha f(x_k)}, \quad k = 0, 1, 2, \ldots \]

(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. \( \square \)

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

4. The method (8) with constant $\alpha$

Consider the selection of the parameter $\alpha$ 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 $\alpha$. Therefore, if the second derivative $f''$ is bounded, there is an $\alpha < 0$ satisfying (27). A positive $\alpha$ 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] $\alpha$.

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

\[ F_{\theta,-1} = \{a (x-\theta) + b (x-\theta)^2 : a, b \in \mathbb{R}\}. \]

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

\[ x_{k+1} = x_k - \frac{(x_k-\theta) f(x_k)}{(x_k-\theta) f'(x_k) - f(x_k)}, \]

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

\[ \hat{f}(x) = \frac{f(x)}{x-\theta} \]

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

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

\[ x_{k+1} = x_k - \frac{(x_k-x_{k-1}) f(x_k)}{(x_k-x_{k-1}) f'(x_k) - f(x_k)}, \quad k = 0, 1, 2, \ldots \]

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 $\zeta$ and $x_1$. Thus to apply (31) it is required to know on which side of $x_0$ lies $\zeta$. 
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
\[
f_1(x) := x^{1/3}
\]
of Example 1. The table below gives a selected iterate \(x_k\) for various combinations of \(x_0\) and \(x_{-1} \).

<table>
<thead>
<tr>
<th>(x_{-1})</th>
<th>(x_0)</th>
<th>(x_1)</th>
<th>(x_2)</th>
<th>(x_3)</th>
<th>(x_4)</th>
<th>(x_5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.01</td>
<td>1.0</td>
<td>(x_{10} = 0.901845)</td>
<td>(x_{100} = 0.193404)</td>
<td>1.1</td>
<td>1.2</td>
<td>(x_{20} = -2.31673 \times 10^{-9})</td>
</tr>
</tbody>
</table>

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
\[
f_3(x) := e^{1-x} - 1
\]
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 \(x_0\).

<table>
<thead>
<tr>
<th>(x_{-1})</th>
<th>(x_0)</th>
<th>(x_1)</th>
<th>(x_2)</th>
<th>(x_3)</th>
<th>(x_4)</th>
<th>(x_5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>10</td>
<td>0.0123266</td>
<td>0.681959</td>
<td>0.875605</td>
<td>0.948526</td>
<td>0.978248</td>
</tr>
<tr>
<td>6</td>
<td>4</td>
<td>2.1897</td>
<td>1.17941</td>
<td>1.01489</td>
<td>1.00114</td>
<td>1.00008</td>
</tr>
</tbody>
</table>

**Example 7.** We apply the method (31) to the function
\[
f_4(x) := xe^{-x}
\]
of Example 4. The table below gives a selected iterate \(x_k\) for various combinations of \(x_0\) and \(x_{-1}\).

<table>
<thead>
<tr>
<th>(x_{-1})</th>
<th>(x_0)</th>
<th>(x_1)</th>
<th>(x_2)</th>
<th>(x_3)</th>
<th>(x_4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>2</td>
<td>(x_{10} = 0.733696)</td>
<td>(x_{100} = 2.25589 \times 10^{-15})</td>
<td>2.5</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>(x_{2} = 0)</td>
<td>(x_{x} = 0)</td>
<td>3.5</td>
<td>2</td>
</tr>
<tr>
<td>100</td>
<td>0</td>
<td>(x_{300} = -0.0473647)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Example 8.** ([6, p. 178, Example 4]) We use (31) to find a root of
\[
f(x) := e^{-x} - \sin x
\]
This is the smallest root. There are infinitely many roots lying close to \(\pi, 2\pi, 3\pi, \ldots\) 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 \(2\pi\) we can use (31) with \(x_{-1} = 4\) and \(x_0 = 5\).

<table>
<thead>
<tr>
<th>(x_{-1})</th>
<th>(x_0)</th>
<th>(x_1)</th>
<th>(x_2)</th>
<th>(x_3)</th>
<th>(x_4)</th>
<th>(x_5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>5</td>
<td>5.76880</td>
<td>6.06502</td>
<td>6.21599</td>
<td>6.25999</td>
<td>6.27596</td>
</tr>
</tbody>
</table>

In contrast, for the same initial \(x_0 = 5\) the Newton method converges to the root closest to \(3\pi\),

<table>
<thead>
<tr>
<th>(x_0)</th>
<th>(x_1)</th>
<th>(x_2)</th>
<th>(x_3)</th>
<th>(x_4)</th>
</tr>
</thead>
</table>

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 \(\theta\)
\[
\mathcal{F}_{\theta, 1} = \left\{ \frac{\alpha}{x-\theta} + b : a, b \in \mathbb{R} \right\}.
\]
The parameter \(\theta\) should be sufficiently far from \(x_0\) for stability reasons. For \(\alpha = 1\) the method (8) gives
\[
x_{k+1} = x_k - \frac{(x_k - \theta) f(x_k)}{f'(x_k) + f(x_k)} - \frac{1}{\theta - \theta} f'(x_k), \quad k = 0, 1, 2, \ldots
\]
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 \( \alpha \) is updated at each iteration. The derivatives of the iteration function of (8)

\[
\Phi_{(8)}(x) := x - \frac{(x - \theta) f(x)}{(x - \theta) f'(x) + \alpha f(x)}
\]

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

\[
\Phi'_{(8)}(\zeta) = 0,
\]

\[
\Phi''_{(8)}(\zeta) = \frac{2 \alpha f'(\zeta) + (\zeta - \theta) f''(\zeta)}{(\zeta - \theta) f'(\zeta)}.
\]

The parameter \( \alpha \) 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

\[
\alpha = -\frac{(\zeta - \theta) f''(\zeta)}{2 f'(\zeta)}
\]

If \( f'' \) is continuous and \( \theta \) is close to \( \zeta \), then (36) can be approximated as

\[
\alpha \approx -\frac{f'(\zeta) - f'(\theta)}{2 f'(\zeta)}
\]

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

\[
\alpha_k := -\frac{f'(x_k) - f'(x_{k-1})}{2 f'(x_k)}.
\]

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

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

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 \( \geq 4.1 \) (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.

<table>
<thead>
<tr>
<th>function</th>
<th>method</th>
<th>initial point(s)</th>
<th>( x_1 )</th>
<th>( x_2 )</th>
<th>( x_3 )</th>
<th>( x_4 )</th>
<th>( x_5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x^{1/3} )</td>
<td>Halley</td>
<td>( x_{-1} = 1, \quad x_0 = 1 )</td>
<td>-0.5</td>
<td>0.25</td>
<td>-0.125</td>
<td>0.0625</td>
<td>-0.0312</td>
</tr>
<tr>
<td></td>
<td>quasi–Halley</td>
<td>( x_{-1} = 1, \quad x_0 = 1 )</td>
<td>-0.559693</td>
<td>1.4699</td>
<td>-0.755481</td>
<td>2.01688</td>
<td>-0.995203</td>
</tr>
<tr>
<td>( x e^{-x} )</td>
<td>Halley</td>
<td>( x_{-1} = 2,1, \quad x_0 = 2 )</td>
<td>4</td>
<td>6.4</td>
<td>8.91177</td>
<td>10.9142</td>
<td>13.0937</td>
</tr>
<tr>
<td></td>
<td>quasi–Halley</td>
<td>( x_{-1} = 2,1, \quad x_0 = 2 )</td>
<td>4.09816</td>
<td>6.82057</td>
<td>4.60104</td>
<td>6.27622</td>
<td>25.7305</td>
</tr>
<tr>
<td>( x^2 - 10 )</td>
<td>Halley</td>
<td>( x_{-1} = 2,5, \quad x_0 = 2 )</td>
<td>2.15384</td>
<td>2.15443</td>
<td>2.15443</td>
<td>2.15443</td>
<td>2.15443</td>
</tr>
<tr>
<td></td>
<td>quasi–Halley</td>
<td>( x_{-1} = 2,5, \quad x_0 = 2 )</td>
<td>2.15238</td>
<td>2.15443</td>
<td>2.15443</td>
<td>2.15443</td>
<td>2.15443</td>
</tr>
<tr>
<td>( e^{-x} - 1 )</td>
<td>Halley</td>
<td>( x_{-1} = 10, \quad x_0 = 10 )</td>
<td>8.00049</td>
<td>6.00013</td>
<td>4.00309</td>
<td>2.21501</td>
<td>1.00018</td>
</tr>
<tr>
<td></td>
<td>quasi–Halley</td>
<td>( x_{-1} = 10, \quad x_0 = 10 )</td>
<td>6.8728</td>
<td>0.357585</td>
<td>0.849521</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( x^4 + 2x^2 )</td>
<td>Halley</td>
<td>( x_{-1} = 1, \quad x_0 = 1 )</td>
<td>0.4</td>
<td>0.135137</td>
<td>0.045055</td>
<td>0.015018</td>
<td>0.005006</td>
</tr>
<tr>
<td></td>
<td>quasi–Halley</td>
<td>( x_{-1} = 1, \quad x_0 = 1 )</td>
<td>0.370739</td>
<td>0.009415</td>
<td>0.002829</td>
<td>0.000943</td>
<td>0.000314</td>
</tr>
</tbody>
</table>
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

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

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

<table>
<thead>
<tr>
<th>iterate</th>
<th>Halley method (x_0 = 3i)</th>
<th>quasi–Halley method (x_{-1} = 1, x_0 = 3i)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(x_1)</td>
<td>(-0.499312 + 2.19129i)</td>
<td>(-0.343620 + 2.52897i)</td>
</tr>
<tr>
<td>(x_2)</td>
<td>(-0.987763 + 1.89479i)</td>
<td>(-1.01552 + 1.84006i)</td>
</tr>
<tr>
<td>(x_3)</td>
<td>(-1.00026 + 1.99934i)</td>
<td>(-1.02212 + 1.97408i)</td>
</tr>
<tr>
<td>(x_4)</td>
<td>(-1 + 2i)</td>
<td>(-0.999892 + 2i)</td>
</tr>
<tr>
<td>(x_5)</td>
<td>(-1 + 2i)</td>
<td></td>
</tr>
</tbody>
</table>

For simple roots of sufficiently smooth functions, the order of convergence of the quasi–Halley method is 2.

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

\[
|x_{k+1} - \zeta| = O\left(|x_k - \zeta|^{1+\sqrt{2}}\right)
\]

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

\[
\Phi_{(38)}(x) = x - \frac{f(x)}{f'(x)} = \frac{f'(x) - f'(x_{k-1})}{2(x - x_{k-1})f'(x)} f(x)
\]

and its second derivative at the zero \(\zeta\) is

\[
\Phi''_{(38)}(\zeta) = \frac{f''(\zeta) - f'\(x_{k-1}\)}{f''(\zeta)} - \frac{f''(\zeta)}{f''(\zeta)} = \frac{f''(\zeta) - f''(\zeta)}{f''(\zeta)}
\]

for some \(\xi\) between \(x_{k-1}\) and \(\zeta\). Since \(f''\) is Lipschitz continuous

\[
|f''(\zeta) - f''(\xi)| \leq L|\zeta - \xi|, \quad \text{for some } L.
\]

(40) \[
\cdot \cdot \cdot \Phi''_{(38)}(\zeta) \leq L |\zeta - \xi| \leq L |x_k - 1 - \zeta| |f'(\zeta)| \leq f'(\zeta).
\]

\[
\cdot \cdot \cdot |x_{k+1} - \zeta| = O\left(|x_k - \zeta|^{1+\sqrt{2}}\right) = O\left(|x_k - \zeta|^{2\gamma+1}\right),
\]

where the order of convergence, \(\gamma\), satisfies the quadratic equation

\[
\gamma^2 - 2\gamma - 1 = 0.
\]

\(\Box\)

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 \(\gamma\) satisfies

\[
1 + \sqrt{2} \leq \gamma < 3.
\]

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

\[
    h_k := \frac{f(x_k)}{f'(x_k) - \frac{f''(x_k)}{2f'(x_k)} f(x_k)}, \quad k = 0, 1, 2, \ldots
\]

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

\[
u_k := \frac{f_k}{f'_k} \quad \text{and} \quad h_k := \frac{f_k}{f'_k - \frac{f''_k}{2f'_k} f_k}.
\]

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

\[
    |f'_k| > \frac{f''_k f_k}{2},
\]

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

\[
    \frac{2}{3} |u_k| \leq |h_k| \leq \frac{4}{3} |u_k|.
\]

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

\[
    q_k := \frac{f(x_k)}{f'(x_k) - \frac{f'(x_k - 1)}{2(x_k - x_{k-1}) f'(x_k)} f(x_k)), \quad k = 0, 1, 2, \ldots
\]

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

\[
    |h_k - q_k| \leq \frac{N}{2 |f_k|} |u_{k-1}|^3.
\]

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

\[
    |h_k - q_k| = O(|h_k|^3),
\]

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


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