Higher order Newton methods: An overview

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Abstract

In this work, we review schemes for solving nonlinear systems of algebraic equations with convergence order larger than two that can be viewed as higher-order extensions of the Newton method, i.e., schemes that only require the function f, its derivative, and an initial guess x_0. We group the schemes into three categories to structure them. The publication is supplemented by an easy-to-use high-accurate Matlab code.

Keywords: algebraic equations, implicit methods, Newton scheme, Potra Ptak, higher-order convergence

1. Introduction

In this publication, we review and group recent (and not so recent) modifications to Newton's method for solving nonlinear equations of form

$$f(\overline{x}) = 0, \tag{1}$$

where f is a vector-valued function $f : \mathbb{R}^n \to \mathbb{R}^n$. The classical Newton method approximates a solution $\overline{x}$ to (1) by a sequence $(x_k)_{k\in\mathbb{N}}$[1], with $x_0 \in \mathbb{R}^n$ given, and x_{k+1} for $k \in \mathbb{N}$ defined through

$$\boxed{x_{k+1} = x_k - f'(x_k)^{-1} f(x_k).} \tag{Newton}$$

Under certain well-established conditions on both f and x_0, one can show that the sequence $(x_k)_{k\in\mathbb{N}}$ converges quadratically to $\overline{x}$, i.e.,

$$\|\overline{x} - x_{k+1}\| \le C\|\overline{x} - x_k\|^2.$$

Already in 1984, Potra and Pták [1] (cited from [2]) have introduced the iterative method

$$\boxed{\begin{aligned} y_k &= x_k - f'(x_k)^{-1} f(x_k) \\ x_{k+1} &= x_k - f'(x_k)^{-1} \left(f(x_k) + f(y_k) \right). \end{aligned}} \tag{PP1984}$$

This method is sometimes called *two-point Newton method with frozen derivative*, see [3], and is a very simple modification of Newton's method that results in third order convergence. In this work, our interest is on extensions of the schemes (Newton) and (PP1984) and related schemes that reach $p-$th order convergence with $p > 2$. Due to efficiency reasons, we restrict ourselves to methods involving at most Jacobians $f'(x)$ (and not any second, third, ... derivatives); and also to methods that can handle $n > 1$ as well.

Please note that this is a survey on recent literature, meaning literature after 2000. As it happens often in research, some methods have been rediscovered and are in turn older methods, see [4] who identify the book by Traub from the 60s [5] as an important source of iterative schemes.

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[1] Please note that for notational convenience, we define $\mathbb{N}$ to be the natural numbers *including* zero.

This paper is equipped with a well-documented Matlab code that can be downloaded as supplementary material. All methods listed in this work are implemented in variable precision arithmetic, such that up to 10,000-digits are taken into account. While this might seem from a practical point of view rather unnecessary, it has the advantage that especially the very high convergence orders can be seen numerically.

We have identified three classes of schemes:

- Forward-quadrature based schemes, see Sec. 2;
- backward-quadrature based schemes, see Sec. 3;
- and generalized methods that can be written in the form of Xiao's schemes [21], see Sec. 4.

The paper's structure is along these three categories.

2. Forward-quadrature-based methods

In this section, we list the various methods that can be found in literature. Many of these methods can be motivated through the observation that the root-finding problem can also be seen as the problem of finding the exact value of an integral. More precisely, for some given x_k, there holds

$$0 \equiv f(\overline{x}) = f(x_k) + \int_0^1 \frac{\mathrm{d}}{\mathrm{d}\tau} f(x_k + \tau(\overline{x} - x_k))\mathrm{d}\tau = f(x_k) + \int_0^1 f'(x_k + \tau(\overline{x} - x_k))\mathrm{d}\tau \cdot (\overline{x} - x_k). \tag{2}$$

Approximating the integral with a suitable method, and replacing the last $\overline{x}$ through x_{k+1}, yields an iteration method. To be more precise, let us consider a generic quadrature formula given by

$$\int_0^1 f'(x_k + \tau(\overline{x} - x_k))\mathrm{d}\tau \approx \sum_{i=1}^{m} \omega_i f'(x_k + \tau_i(\overline{x} - x_k)), \tag{3}$$

where ω are the quadrature weights and τ are the quadrature points. The most obvious way is to set $\tau = \{0\}$ and $\omega = \{1\}$ to obtain

$$0 = f(x_k) + f'(x_k)(\overline{x} - x_k).$$

Replacing $\overline{x}$ by x_{k+1} yields the classical Newton's method (Newton).

In [6], the authors use a general Newton-Cotes formula of order at least one[2]. However, they do not apply it to the integral as it is in (3), but they apply it to the integral where $\overline{x}$ has been replaced by y_k, where y_k is one Newton step with starting value x_k. This has been motivated by earlier works from Weerakoon and Fernando, see [7]. Hence,

$$\int_0^1 f'(x_k + \tau(\overline{x} - x_k))\mathrm{d}\tau \approx \int_0^1 f'(x_k + \tau(y_k - x_k))\mathrm{d}\tau \approx \sum_{i=1}^{m} \omega_i f'(x_k + \tau_i(y_k - x_k)). \tag{4}$$

In combination with (2), this then leads to the class of schemes

$$\boxed{\begin{aligned} y_k &= x_k - f'(x_k)^{-1} f(x_k), \\ x_{k+1} &= x_k - \left(\sum_{i=1}^{m} \omega_i f'(x_k + \tau_i(y_k - x_k))\right)^{-1} f(x_k). \end{aligned}} \tag{FS2003}$$

[2] By 'order one' of a quadrature formula, we mean that both constant and linear functions are exactly integrated. In this setting, where $\int_0^1 \ldots \mathrm{d}\tau$ is approximated, this comes down to the requirement that $\sum_{i=1}^m \omega_i = 1$ and $\sum_{i=1}^m \omega_i \tau_i = \frac{1}{2}$. The quadrature rule that can be used to derive Newton's method ($m = 1$, $\omega_1 = 1$ and $\tau_1 = 0$) only integrates constants correctly, and hence does not fall into this scope.

ω	τ	Order	Abbreviation	Ref
$\left\{\frac{1}{2}, \frac{1}{2}\right\}$	$\{0, 1\}$	3	WF2000	[7, 10, 11]
$\{1\}$	$\left\{\frac{1}{2}\right\}$	3	CT2006(2)	[10, 8, 9]
$\left\{\frac{1}{6}, \frac{4}{6}, \frac{1}{6}\right\}$	$\left\{0, \frac{1}{2}, 1\right\}$	3	CT2007(1)	[12, 13]
$\left\{\frac{2}{3}, -\frac{1}{3}, \frac{2}{3}\right\}$	$\left\{\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right\}$	3	CT2007(2)	[12, 13]
$\left\{\frac{1}{4}, \frac{3}{4}\right\}$	$\left\{0, \frac{2}{3}\right\}$	3	NW2009	[14]
$\{1 - \beta, \beta\}$	$\left\{0, \frac{1}{2\beta}\right\}$	3	Wang2011	[15]
$\left\{\frac{1}{2}, \frac{1}{2}\right\}$	$\left\{\frac{1}{3}, \frac{2}{3}\right\}$	3	Khi2012(1)	[13]
$\left\{\frac{1}{8}, \frac{3}{8}, \frac{3}{8}, \frac{1}{8}\right\}$	$\left\{0, \frac{1}{3}, \frac{2}{3}, 1\right\}$	3	Khi2012(2)	[13]
$\left\{\frac{1}{2}, \frac{1}{2}\right\}$	$\left\{\frac{1}{2} - \frac{1}{2\sqrt{3}}, \frac{1}{2} + \frac{1}{2\sqrt{3}}\right\}$	3	LZH2016(1)	[16]
$\left\{\frac{8}{18}, \frac{5}{18}, \frac{5}{18}\right\}$	$\left\{\frac{1}{2}, \frac{1}{2} \mp \frac{\sqrt{3}}{2\sqrt{5}}\right\}$	3	Noor2018	[17]
$\left\{\frac{1}{2}, \frac{1}{2}\right\}$	$\left\{\frac{1}{4}, \frac{3}{4}\right\}$	3	MPD2021(1)	[35]

Table 1: List of schemes based on the quadrature formula (FS2003). The iterations $x_{k+1} = \dots$ can be derived by putting ω and τ into (FS2003). For Wang2011, β is a real-valued parameter; for $\beta = 1$, one recovers CT2006(2), for $\beta = \frac{1}{2}$, one recovers WF2000, for $\beta = \frac{3}{4}$, one recovers NW2009. Please note that 'order' denotes order of convergence (if convergence occurs) for generic f. For special f and, e.g., double roots or the like, it can be more or less. For details, consult (FS2003).

This class of schemes is called *mNm* (modified Newton method); different schemes can be obtained for different choices of ω_i and τ_i. In literature, we have found plenty of choices, see Tbl. 1. It has to be noted that not all schemes listed in the table were originally designed to follow the paradigm laid out here. E.g., in [8, 9], a third-order scheme is developed based on the general class of schemes

$$y_k = x_k - a(x_k)f(x_k), \qquad x_{k+1} = x_k - f'(y_k)^{-1}f(x_k).$$

It is observed that this converges cubically for the choice $a(x_k) = \frac{1}{2}f'(x_k)^{-1}$ (amongst others). It is an easy exercise to show that this method coincides with the mid-point Newton method CT2006(2).

One might be tempted to hope that with increasing m, i.e., with a better integral approximation, the order of the scheme improves. However, it is shown in [6] that the order can not exceed three, see [6, Thm. 1]. In fact, if the quadrature rule is of order one at least, it will always be cubically convergent under mild conditions on f and sufficient closedness of x_0 to $\overline{x}$. While the work in [6] is on scalar equations, it is extended in [18] to systems of equations.

One way to obtain higher order convergence is through combining schemes. Let $z_k := \Phi_{PP}(x_k)$ be the action of the third-order scheme (PP1984) on x_k. Then, one can substitute $\overline{x}$ in (4) not by y_k, but by z_k. This has been realized by Darvishi and Barati [19], and, together with the Simpson rule, leads to the fourth-order scheme

$$\boxed{\begin{aligned} z_k &= \Phi_{PP}(x_k), \\ x_{k+1} &= x_k - \left(\frac{1}{6}f'(x_k) + \frac{2}{3}f'\left(\frac{x_k + z_k}{2}\right) + \frac{1}{6}f'(z_k)\right)^{-1} f(x_k) \end{aligned}} \tag{DB2007}$$

3. Backward-quadrature-based methods

In [20], it is not the function f that is expanded in an integral as in (2), but the inverse function f^{-1} (that is assumed to exist locally). For this function, there obviously holds $f^{-1}(0) = \overline{x}$, and

$$\overline{x} \equiv f^{-1}(0) = x_k + \int_0^1 (f^{-1})'(f(x_k) + \tau(0 - f(x_k)))\mathrm{d}\tau \cdot (0 - f(x_k)).$$

Again, using a Newton-Cotes of order at least one, one obtains

$$\overline{x} \approx x_k + \sum_{i=1}^{m} \omega_i (f^{-1})'(f(x_k) + \tau_i(0 - f(x_k))) \cdot (0 - f(x_k)).$$

Combined with the rule for differentiation of inverses, $(f^{-1})'(y) = \left(f'(f^{-1}(y))\right)^{-1}$, there holds

$$\overline{x} \approx x_k - \sum_{i=1}^{m} \omega_i f'(f^{-1}((1-\tau_i)f(x_k)))^{-1} \cdot f(x_k).$$

To make this computable, the authors in [20] now assume that the behavior of f is locally linear, i.e., $f(x) = f(x_k) + f'(x_k)(x - x_k)$, which implies that the inverse function is given by $f^{-1}(y) = f'(x_k)^{-1}(y - f(x_k)) + x_k$. Note that under this assumption, $f^{-1}((1-\tau_i)f(x_k)) = x_k - \tau_i f'(x_k)^{-1} f(x_k)$. Ultimately, this then yields the final scheme given by

$$\boxed{\begin{aligned} y_k^{(i)} &= x_k - \tau_i f'(x_k)^{-1} f(x_k), \quad 1 \leq i \leq m, \\ x_{k+1} &= x_k - \sum_{i=1}^{m} \omega_i f'(y_k^{(i)})^{-1} f(x_k). \end{aligned}} \tag{HH2005}$$

The scheme is of order three (and not more) under mild conditions on f and x_0, as long as the Newton-Cotes formula used is exact to at least degree one.

There are schemes that are somewhere in-between the forward and the backward quadrature schemes, and cannot naturally be listed under the general formulation in the next section. The schemes we identified in this respect are the one by Cordero, Hueso, Torregrosa, Martinez (2010) [32], the sixth-order scheme

$$\boxed{\begin{aligned} y_k &= x_k - \frac{2}{3} f'(x_k)^{-1} f(x_k), \\ z_k &= x_k - \frac{1}{2} \left(3f'(y_k) - f'(x_k)\right)^{-1} \left(3f'(y_k) + f'(x_k)\right) f'(x_k)^{-1} f(x_k) \\ x_{k+1} &= z_k - \left(-\frac{1}{2} f'(x_k) + \frac{3}{2} f'(y_k)\right)^{-1} f(z_k) \end{aligned}} \tag{CHTM2010}$$

and the fourth-order one by Grau-Sanchez, Grau and Noguera (2011) [33],

$$\boxed{\begin{aligned} y_k &= x_k - f'(x_k)^{-1} f(x_k), \\ z_k &= y_k - \frac{1}{2} f'(x_k)^{-1} f(y_k) \\ x_{k+1} &= y_k - 2f'(x_k)^{-1} f(z_k). \end{aligned}} \tag{GGN2011(1)}$$

4. Generalized methods

In 2022, Xiao [21] has introduced the very general class of schemes that tries to unify several schemes found in literature. It is assumed that a certain scheme of order p, denoted through Φ, is given[3] . Then, the class of schemes introduced in [21] reads

$$\boxed{\begin{aligned} y_k &= x_k - a f'(x_k)^{-1} f(x_k) \\ z_k &= \Phi(x_k, y_k) \\ x_{k+1} &= z_k - \left(b\mathcal{I} + c f'(y_k)^{-1} f'(x_k) + d f'(x_k)^{-1} f'(y_k)\right) f'(x_k)^{-1} f(z_k) \end{aligned}} \tag{Xi2022}$$

[3] In [21], $p \geq 2$ is assumed. For this presentation, this is not required.

$[a,b,c,d]$	$\Phi(x,y)$	Order	Abbreviation	Ref
$[1,0,0,0]$	$x - \frac{1}{2} f'(y)^{-1} f'(x)^{-1} \left(f'(x) + f'(y)\right) f(x)$	2	CT2006(1)	[10, 22]
$[1,0,1,0]$	y	4	Chun2006	[23]
$[\beta,0,0,0]$	$x - \left(\mathcal{I} + \frac{1}{2\beta}\left(\mathcal{I} - \frac{\lambda}{\beta}\left(\mathcal{I} - f'(x)^{-1} f'(y)\right)\right)^{-1}\left(\mathcal{I} - f'(x)^{-1} f'(y)\right)\right) f'(x)^{-1} f(x)$	$3/4^{*}$	Ne2008	[24, 25]
$[1,2,0,-1]$	y	4	CMT2009(1)	[26]
$[1,0,1,0]$	$\Phi(x,y)^{**}$	$p+2$	CHMT2012	[27, 28]
$[\theta,a_1,a_2,a_3]$	x	4^{***}	SGS2013	[29]
$[\frac{2}{3},0,0,0]$	$x - \left(\frac{23}{8}\mathcal{I} - f'(x)^{-1} f'(y)\left(3\mathcal{I} - \frac{9}{8} f'(x)^{-1} f'(y)\right)\right) f'(x)^{-1} f(x)$	4	SA2014(1)	[30]
$[\frac{2}{3},\frac{5}{2},0,\frac{-3}{2}]$	$x - \left(\frac{23}{8}\mathcal{I} - f'(x)^{-1} f'(y)\left(3\mathcal{I} - \frac{9}{8} f'(x)^{-1} f'(y)\right)\right) f'(x)^{-1} f(x)$	6	SA2014(2)	[30]
$[\frac{1}{2},-1,2,0]$	$x - f'(y)^{-1} f(x)$	5	SG2014	[31]
$[1,0,1,0]$	$\Phi_{LZH2016(1)}(x,y)$	5	LZH2016(2)	[16]
$[1,0,1,0]$	$\Phi_{MPD2021(1)}(x,y)$	5	MPD2021(2)	[35]

Table 2: List of schemes based on the general formula introduced in [21], see (Xi2022). $\mathcal{I}$ denotes the identity matrix. For the definition of $\Phi_{LZH2016(1)}$ and $\Phi_{MPD2021(1)}$, consult Tbl. 1. Please note that 'order' denotes order of convergence (if convergence occurs) for generic f. For special f and, e.g., double roots or the like, it can be more or less. For details, consult (**??**).
*: Order 3 for any choice of λ and β, and order four for $\lambda = 1$ and $\beta = \frac{2}{3}$.
**: Φ is an arbitrary iteration scheme of order p.
***: For the choice of the values $a_1 = -\frac{1}{2}$, $a_2 = \frac{9}{8}$, $a_3 = \frac{3}{8}$ and $\theta = \frac{2}{3}$.

It is shown in [21] that this scheme, given that Φ is of order $p \geq 2$, is of order $p+3$ iff $a = 1$, $b = -1$, $c = \frac{3}{2}$ and $d = \frac{1}{2}$, again under mild conditions on f and x_0. Furthermore, it is shown that the scheme is of order $p+2$, if there holds

$$b + c + d = 1, \qquad a(c-d) = 1.$$

In Tbl. 2, we have listed methods from literature that can be rather naturally cast into this form.

Remark 1. *Please note that due to the term $z_k = \Phi(x_k, y_k)$,* any *scheme that can be written in form $x_{k+1} = \Psi(x_k)$ (so all the schemes shown here so far) can be cast into this framework through the obvious definition $[a,b,c,d] = [0,0,0,0]$, and $\Phi(x_k, y_k) := \Psi(x_k)$. However, for some schemes it is more natural to do this than for others, see Tbl. 2.*

5. Conclusions

In this work, we have listed several higher-order extensions of Newton's method that have been published within roughly the last two decades. During our literature study, we came across many more works on related concepts. Some interesting facts are listed below, without the intention to be anything near a complete list – the field is vast.

- The schemes in [36] do not work for $n > 1$ and are hence not listed here. However, we think that this paper is very interesting, as it gives in Table 1 a very nice overview over other derivative-free iteration methods for functions $f : \mathbb{R} \to \mathbb{R}$.
- Some schemes make heavy use of the concept of multivariate divided differences, see, e.g., [3, 37, 38]. We have not included them in this overview here as in the applications we have in mind, the inverse is not computed explicitly, but its action on a certain vector is computed through a matrix-free Newton-Krylov scheme. Derivatives are hence avoided at all.

- In the quadrature-based approaches as seen in Sec. 2–3, the value of the unknown point $\overline{x}$ is approximated by a standard Newton step. This can obviously also be replaced by a Halley step, involving second derivatives of f. For an example, see, e.g., [39].
- We did not take into account the schemes presented in [34], as they seemed to be very difficult in their formulation. Amongst others, they involve $f'(x_k)^{-3}$, which is rather impractical in our applications.
- Another interesting field of research is iterative schemes through Adomian decomposition, see, e.g., [23]. Here, the unknown $\overline{x}$ and the function are decomposed into series (for the function a series of Adomian's polynomials). This also yields high-order schemes of increasing complexity.

None of the content in this work is new. We hope, however, that this literature overview and the classification can be of use to some wanting to try schemes beyond Newton's scheme.

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