The Systematic Formation of High-Order Iterative Methods

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Abstract

Fixed point iteration and the Taylor-Lagrange formula are used to derive, some new, efficient, high-order, up to octic, methods to iteratively locate the root, simple or multiple, of a nonlinear equation. These methods are then systematically modified to account for root multiplicities greater than one. Also derived, are super-quadratic methods that converge contrarily, and super-linear and super-cubic methods that converge alteratingly, enabling us, not only to approach the root, but also to actually bound and bracket it.

Keywords: Fixed point iteration; The generation of high order iterative functions; The Taylor-Lagrange formula; High-order iterative methods; Undetermined coefficients; Contrary and alternating convergence; Root bracketing

Fixed Point Iteration

Consider the paradigmatic fixed point iteration
\[ x_i = F(x_{i-1}) \] (1)
to locate fixed point a, F(a)=a of contracting function F(x). We write \( x_i - a = F(x_i) - a \) and have by power series expansion that
\[ x_i - a = F'(a)(x_i - a) + \frac{1}{2!} F''(a)(x_i - a)^2 + \frac{1}{3!} F'''(a)(x_i - a)^3 + \ldots \] (2)
implying that if 0<|F'(x)|<1 near x=a, namely, if F(x) is indeed contracting, then the fixed point iteration converges linearly, and if F'(a)=0, then the fixed point iteration converges quadratically, and so on.

Suppose now that we are seeking root a, f(a)=0, f'(a) ≠ 0, of function f(x). To secure a quadratic iterative method we rewrite f(x)=0 as the equivalent fixed point problem
\[ x = F(x), \quad F(x) = x + w(x)f(x) \] (3)
for weight function w(x),w(a) ≠ 0, which we seek to fix to our advantage.

For a quadratic method we need w(x) to be such that
\[ F'(a) = 0, \quad f'(a) ≠ 0 \]
requiring w(x)=−f'(a)/f''(a), and w(a)=−1/f''(a), which is actually quadratic
\[ x_i - a = \frac{f'}{2f''}(x_i - a)^2 + o((x_i - a)^3) \] (6)
where f'=f(a) ≠ 0, f''=f''(a) < ∞, and where x_i is the iterative input and x the iterative output.

From the two zero conditions
\[ F(x) = f(x) + f'(x)w(x) = 0, \quad F'(x) = f'(x) + f'(x)w'(x) + f(x)w'(x) = 0 \] (7)
we obtain, after ignoring f(x) w'(x) in the second of equations (7), the system of equations
\[
\begin{bmatrix}
  f' & f \\
  f' & 2f''
\end{bmatrix}
\begin{bmatrix}
w \\
w'
\end{bmatrix}
= \begin{bmatrix}
-1 \\
0
\end{bmatrix}
\] (8)
which we solve for w(x) as
\[
w = \frac{\begin{vmatrix}
-1 & f \\
0 & 2f''
\end{vmatrix}}{\begin{vmatrix}
f' & f \\
f' & 2f''
\end{vmatrix}} = \frac{f''}{f - f'} \]
(9)
to have Halley’s method
\[
x_i = x_{i-1} - \frac{f(x_{i-1}) - f'(x_{i-1})w(x_{i-1})}{f'(x_{i-1}) - f''(x_{i-1})w'(x_{i-1})} = x_{i-1} - \frac{1}{2}f'(x_{i-1})w_{i-1} = \frac{x_{i-1} - f'(x_{i-1})}{2f''(x_{i-1})} \]
which is, indeed, cubic
\[
x_i - a = \frac{1}{12} f^{(2)}(x_{i-1})w(x_{i-1}) + o((x_{i-1} - a)^4) \]
(11)
provided that f(a)=0, but f'(a) ≠ 0.

Requesting that f(a)=a, F(a)=0, F'(a)=0, F''(a)=0, we similarly obtain the method
\[
x_i = x_{i-1} + \frac{1}{f''(x_{i-1})} \frac{f(x_{i-1}) - f'(x_{i-1})w(x_{i-1})}{f'(x_{i-1}) - f''(x_{i-1})w'(x_{i-1})} = x_{i-1} + \frac{1}{2}f'(x_{i-1})w_{i-1} \]
(12)
which is quartic
\[
x_i - a = \frac{1}{12} f^{(2)}(x_{i-1})w(x_{i-1}) + o((x_{i-1} - a)^4) \]
(13)
provided that f=0 ≠ 0.

Higher order single-point methods are readily obtained by

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requesting higher order derivatives of \( F(x) = x + w(x) \) \( f(x) \) to to zero at \( x = a, f(a) = 0 \) \[1\].

**A Recursive Determination of the Higher Order Iterative Function**

There are various ways to recursively generate a new higher order iterative function \( F(x) \) of eq. (1) from a known lower order one. Traub [2] has suggested such a rational recursive formula. If, for example, \( F(x) = F_2(x) \) is such that

\[
F_2'(a) = 0, \quad F_2(a) = 0
\]

then

\[
F_2(x) = \frac{n F_1(x) - x F_2'(x)}{n-F_2'(x)}, n = 2
\]

is such that

\[
F_2(a) = a, F_2'(a) = 0, F_2''(a) = 0
\]

with which the iterative method \( x_1 = F_2(x_0) \) to locate fixed point \( a, F(a) = a \) becomes cubic

\[
x_1 - a = -\frac{1}{12} F''(a)(x_0 - a)^3 + O((x_0 - a)^4).
\]

Instead of rational formula (15) we suggest the product formula

\[
F_3(x) = F_2(x) + \frac{1}{n} F_2(F_2' - x), n = 2
\]

which is, indeed, cubic

\[
x_1 - a = -\frac{1}{6} (2F''(a)^3 - F'''(a)) (x_0 - a)^3 + O((x_0 - a)^4).
\]

For example, for Newton’s method \( F_2(x) = x - f(x)/f'(x) \). Using formula (18) we obtain by it the method

\[
x_1 = F_3(x_0), F_3(x_0) = x_0 - u_0 - \frac{f'''}{2f''} u_0^2, \quad u_0 = \frac{f_0}{f''}
\]

which is, indeed, cubic

\[
x_1 - a = -\frac{1}{6} f'' + f''' (x_0 - a)^3 + O((x_0 - a)^4).
\]

provided that \( f'''(a) \neq 0 \).

Iterative method (20) is also obtained from Halley’s method of eq. (10) using the approximation

\[
(1 - \frac{f'''}{2f''} u_0) = 1 + \frac{f'''}{2f''} u_0.
\]

Further, if \( F_3(x) \) is such that

\[
F_3'(a) = a, F_3'(a) = 0, F_3''(a) = 0
\]

then

\[
F_{n+1}(x) = F_3 + \frac{1}{n} F_3(F_3' - x), n = 3
\]

is such that

\[
F_3(a) = a, F_3'(a) = 0, F_3''(a) = 0
\]

and the iterative method \( x_1 = F_3(x_0) \) to locate fixed point \( a \) is quartic

\[
x_1 - a = -\frac{1}{72} F^{(4)}(x_0 - a)^4 + O((x_0 - a)^5).
\]

It is well known that the modified Newton’s method

\[
x_1 = F_3(x_0), F_2(x) = x - m \frac{f(x)}{f'(x)}
\]

converges quadratically to a root of any multiplicity \( m \geq 1 \). From equation (24) we derive the third order method

\[
x_1 = F_3(x_0), F_3(x) = x - \frac{1}{2} m(3 - m) u - m^2 \frac{f'''}{2f''} u^2, u = \frac{f(x)}{f'(x)}
\]

Indeed, assuming that

\[
f(x) = (x - a)^n g(x), \quad g(a) \neq 0
\]

we obtain for the method in eq. (28)

\[
x_1 - a = \frac{(3 + m)B^2 - mAC}{2m^2 A^2} (x_0 - a)^3 + O((x_0 - a)^4)
\]

where \( A = g(a), B = g'(a), C = g''(a) \), and \( m \) is the multiplicity index of repeating root \( a \) [3].

From eq. (29) we have

\[
\left( \frac{f(x)}{f'(x)} \right)' = -\frac{2}{m} \frac{g'(a)}{g(a)} (x - a) + O((x - a)^2)
\]

by which we may, knowing an \( x \) close to \( a \), estimate \( m \).

**A One-Sided Third-Order Two-Step, or Chord, Method**

Having computed \( x_1 = x_0 - f_0/f''_0 \) we return to correct it as the midpoint method

\[
x_2 = x_0 - \frac{f(x_0)}{f''(x_0/2)} = x_0 - \frac{f(x_0)}{f''(x_0/2) u_0}, u_0 = \frac{f_0}{f''}
\]

which is now cubic, or third order

\[
x_2 - a = \frac{6 f'''}{24 f''} (x_0 - a)^3 + O((x_0 - a)^4).
\]

See also Traub [2] page 164 eq. (8-12).

The modified method

\[
x_2 = x_0 - \frac{4 f_0}{f'' + 3 f''(x_0 - 2u_0)}
\]

is cubic

\[
x_2 - a = \frac{1}{4} \frac{f'''}{f''} (x_0 - a)^3 + O((x_0 - a)^4)
\]

and one sided. At least asymptotically, if \( x_0 - a > 0 \), then also \( x_2 - a > 0 \), and if \( x_0 - a < 0 \), then also \( x_2 - a < 0 \).

Using the approximation

\[
f'(x - \frac{1}{2} u) = \frac{f(x) - f(x - u)}{u}
\]

equation (32) becomes the two-step, or chord, method

\[
x_2 = x_0 - \frac{f(x_0)}{f''(x_0/2)} = x_0 - \frac{f(x_0)}{f''(x_0/2) u_0}, u_0 = \frac{f_0}{f''}
\]

where \( u_0 = f_0 / f'' \). \( x_1 = x_0 - u_0 f'(x_0) \). All three methods of eq. (37) are cubic

\[
x_2 - a = \frac{1}{4} \frac{f'''}{f''} (x_0 - a)^3 + O((x_0 - a)^4)
\]

See Traub [2-4].

Convergence of this method is also one sided.
Construction of High-Order Iterations by Undetermined Coefficients

Halley’s method, or for that matter any other higher order method, can be constructed by writing \( \delta x, x_1 = x_0 + \delta x \), as a power series of \( u_0 = f_0/f' \), or even of merely \( f_0 = f(x_0) \). For example, we write the quadratic
\[
2
f_0^2 + f_0 + Qf_0 = 0,
\]
and then sequentially fix the undetermined coefficients \( P \) and \( Q \) for highest attainable order of convergence.

Thus, at first we have from eq. (39) that
\[
x_1 - a = \left(1 + P f'\right)(x_0 - a) + O((x_0 - a)^3),
\]
and we set \( a = -1/f' \). With this \( P \) we have next that
\[
x_2 - a = \left(f' + f''Q\right)(x_0 - a)^2 + O((x_0 - a)^3),
\]
and we set
\[
P = \frac{-1}{f'}, \quad Q = \frac{f'}{2f''},
\]
with which the polynomial method of eq. (20) is recovered.

Doing the same to the rational method
\[
x_1 - a = \left(1 + P f\right)(x_0 - a) + O((x_0 - a)^3),
\]
we determine by power series expansion that cubic convergence is assured for \( P = -1/f_0, Q = 0, R = 1, S = -f''/(2f'f_0) \), with which the classical Halley’s method of eq. (10) is recovered.

Quartic and Quintic Multistep Methods

The rational two-step method (a generalization of the method in eq. (37)) of Ostrowski [5] appendix G,
\[
x_1 - a = \frac{1}{2} f' \left(3 f'^2 - 2 f f''\right) + O((x_0 - a)^3),
\]
and Traub [2,3,6-8]
See also page 184 eq. (8-78).

The polynomial in \( r \) method
\[
x_1 - a = \frac{1}{2} f' \left(3 f'^2 - 2 f f''\right) + O((x_0 - a)^3),
\]
is as follows:
\[
x_2 - a = \frac{1}{2} f' \left(3 f'^2 - 2 f f''\right) + O((x_0 - a)^3).
\]
The multistep method
\[
x_1 = x_0 - \frac{1}{1-r} f_0, \quad x_1 = x_0 - \frac{1-r}{1-2r} f_0, \quad r = \frac{f_1}{f_0}, \quad u_0 = \frac{f_0}{f_0}
\]
is quantic.

Sextic and Octic Multistep Methods

The multistep method
\[
x_2 = x_0 - (1 + r + 2r^2) u_0, \quad x_2 = x_0 - \frac{1-r}{1+3r} f_0, \quad r = \frac{f_1}{f_0}, \quad u_0 = \frac{f_0}{f_0}
\]
is sextic.

We set
\[
x_3 - a = \frac{1}{144} f' \left(-15 f'^2 + 2 f f''\right) + O((x_0 - a)^3).
\]
The method
\[
x_2 = x_0 - \frac{f(1+x)}{g'}, \quad g' = \left(1 - 2r + 3r^2 - s(1+2r^2)\right)f', \quad r = \frac{f_1}{f_0}, \quad s = \frac{f_0}{f_1},
\]
is octic.

Contrarily converging super-quadratic methods

We write
\[
x_1 = x_0 - \frac{1}{2} f' (x_0 - a)^2 + O((x_0 - a)^3),
\]
for undetermined coefficient \( P \), and have
\[
x_2 - a = \frac{1}{2} f' \left(1-P\right)(x_0 - a)^2 + O((x_0 - a)^3).
\]
We request that
\[
f' \left(1-P\right) = 2k\left(f'/f_0\right)^2
\]
for parameter \( k \), by which the iterative method in eq. (54) turns into
\[
x_2 = x_0 - \frac{1}{1-k} f_0 + 4kr^2
\]
for any constant \( k \), and
\[
x_2 - a = k\left(f'/f_0\right)^2 (x_0 - a)^2 + O((x_0 - a)^3).
\]
This super-quadratic method converges from above if \( k > 0 \), and from below if \( k < 0 \).

The interest in the method
\[
x_2 = x_0 - \frac{1}{1-r} u_0, \quad x_1 = x_0 - u_0, \quad f_1 = f(x_1), \quad r = \frac{f_1}{f_0}, \quad u_0 = \frac{f_0}{f_0}
\]
is that it ultimately converges oppositely to Newton’s method,
\[
x_2 - a = \frac{1}{2} f' (x_0 - a)^2 + O((x_0 - a)^3),
\]
as is seen by comparing eq. (60) with eq. (6).

The average of Newton’s method and the method of eq. (59) is cubic,
\[
\frac{1}{2} (x_0 + x_0) - a = \frac{1}{6} f' (x_0 - a)^2 + O((x_0 - a)^3).
\]

Alternatingly Converging Super-Linear and Super-Cubic Methods

We start by modifying Newton’s method
\[
x_i = x_0 - (1+k) f_k, \quad k \geq 0
\]
to have
\[
x_i - a = k(x_0 - a) + O((x_0 - a)^3)
\]
indicating that, invariably, the method converges, at least asymptotically,
alternating. For \( k > 0 \), if \( x_n - a > 0 \), then \( x_n - a < 0 \), and vice versa. For
a higher-order alternating method we rewrite the originally quartic method
of eq. (46) as
\[
x_2 = x_0 - (1 + r + Qr^2)u_n, \quad u_n = \frac{f_n}{f_0}, \quad r = \frac{f_n}{f_0}, \quad f_1 = f(x_0 - u_n)
\]
for the undetermined coefficient \( P \), and have that for a root of multiplicity

\[
x_2 - a = -k \left( \frac{f_n}{f_0} \right)^2 (x_n - a)^2 + O((x_n - a)^4), \quad k = \frac{1}{4}(Q - 2).
\]

This super cubic method converges alternatingly if parameter \( k > 0 \).

**Correction for Multiple Roots by Undetermined Coefficients**

We rewrite Newton’s method as
\[
x_1 = x - Pu_0, \quad u_0 = \frac{f_0}{f_0}
\]
for undetermined coefficient \( P \), and have that for a root of multiplicity \( m \geq 1 \)
\[
x_1 - a = \left( 1 - \frac{P}{m} \right) (x_n - a) + \frac{P \cdot B}{m^2 A} (x_n - a)^2 + O((x_n - a)^3)
\]
where \( A=g(a), B=g'(a) \) for \( g(x) \) in eq. (29). Quadratic convergence is
restored, as is well known, with \( P=m \).

With \( P=m(1-k), k<0 \) the modified Newton’s method of eq. (66)

\[
\delta x = \frac{f_0'}{f_0} \delta x + \frac{f_0''}{2f_0} \delta x^2 + \ldots
\]
and take \( f(x_0+\epsilon x)=0, \xi=x_0 \) to obtain the iterative method

\[
x_2 = x_0 + \delta x, \quad f_2 = f(x_0) + \delta x f'_0(x_0) + \frac{1}{2} \delta x^2 f''_0(x_0).
\]

We approximate the solution of the increment equation
\[
f_0 + \delta x f'_0 + \frac{1}{2} \delta x^2 f''_0 = 0
\]
or, for that matter, any such higher order algebraic equation, by the
power series
\[
\delta x = (P + Qf'_0 + Rf''_0 + Sf'''_0 + \ldots)f_0
\]
and have upon substitution and collection that
\[
(1 + Pf'_0 + (Qf'_0)^2 f''_0 + (Rf''_0 + P(f''_0))^3 + (Sf'''_0 + \frac{1}{2} Qf''_0 + Rf''_0)) = 0
\]
and we may have that
\[
p = \frac{1}{2} f''_0, \quad R = -PQf'_0, \quad S = -Q^2Pf''_0 + PPSf''_0, T = -(QP + PS)f''_0
\]
where \( s=f''/f_0 \).

The methods
\[
x_1 = x_0 + P f'_0 + Q f''_0 + R f'''_0
\]
and \( x_1 = x_0 + P f'_0 + Q f''_0 + R f'''_0 \) are both cubic
\[
x_1 - a = \frac{1}{6} \frac{1}{(x_n - a)^3} + O((x_n - a)^4)
\]
provided that \( f'(a) \neq 0 \).

The method
\[
x_1 = x_0 - (P + Qf'_0 + Rf''_0 + S(f''_0 + 1 + f''_0 u_n) u_n) = f_0 f''_0 f''_0 f''_0 = -f_0 f''_0 f''_0 f''_0 f''_0
\]
converges cubically as well to a root of any multiplicity \( m \geq 1 \)
\[
x_1 - a = \frac{3}{2} \frac{B^2 - 2mAC}{2m^2 A^2} (x_0 - a)^3 + O((x_0 - a)^4)
\]
where \( A=g(a), B=g'(a), C=g''(a) \) for \( g(x) \) in eq. (29) [11-13].

**Still Higher Order Methods**

Starting with
\[
f(x) = f(x_0 + \delta x) = f_0 + \delta x f'_0 + \frac{1}{2} \delta x^2 f''_0 + \frac{1}{6} \delta x^3 f'''_0 + \ldots
\]
we obtain the iterative method

\[
x_1 = x_0 + \delta x, \quad f_1 = f_0 + \delta x f'_0 + \frac{1}{2} \delta x^2 f''_0 + \frac{1}{6} \delta x^3 f'''_0 = 0
\]
with
\[
\delta x = (P + Qf'_0 + Rf''_0 + Sf'''_0 + \ldots)f_0
\]
The methods
\[ x_i = x_0 + (P + Qf'_0 + Rf''_0) f_0 \] and
\[ x_2 = x_0 + (P + Qf'_0 + Rf''_0 + Sf'''_0) f_0 \]
are both quartic
\[ x_2 - a = \frac{1}{24} \frac{f'''}{f'} (x_0 - a)^4 + O((x_0 - a)^5) \]
provided that \( f'(a) \neq 0 \).

**Unknown Root Multiplicity**

The two single-step methods
\[ x_1 = x_0 - m \frac{f_0}{f_0'}, \ x_2 = x_0 + \frac{f_0'}{f'_0} f_0 \]
converge contrarily to root \( a \) of any multiplicity \( m \)
\[ x_i - a = -\frac{1}{m} A (x_i - a)^2 + O((x_i - a)^3) \]
where \( A = g(a) \), \( B = g'(a) \) for \( g(x) \) in eq. (29). Their average is a cubic method
\[ x_i - a = \frac{B'(m-1) - 2ACm}{2Am^2} (x_i - a)^3 + O((x_i - a)^4) \]
where \( A = g(a), B = g'(a), C = g''(a) \) for \( g(x) \) in eq. (29).

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