A Symbolic and Numerical Exploration of a High-Order Newton Method

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Taylor Expansion and Initial Approximation

Let $a_p = \frac{f^{(p)}(x_0)}{p!}$.

Assume $x = c$, and $f(x) = f(c) = 0$.

The Taylor expansion of $f(x)$ about $x = x_0$ is:

$$f(x) = a_0 + a_1 h + a_2 h^2 + a_3 h^3 + a_4 h^4 + \cdots$$

Since $f(c) = 0$, we rearrange:

$$0 = a_0 + a_1 h + a_2 h^2 + a_3 h^3 + a_4 h^4 + \cdots$$

$$a_0 = -(a_1 h + a_2 h^2 + a_3 h^3 + a_4 h^4 + \cdots)$$

Now divide both sides by $a_1 h$:

$$-\frac{a_0}{a_1 h} = 1 + \frac{a_2}{a_1} h + \frac{a_3}{a_1} h^2 + \frac{a_4}{a_1} h^3 + O(h^4)$$

Taking the reciprocal:

$$\frac{1}{a_0} = -\frac{1}{a_1 h}\left(1 + \frac{a_2}{a_1} h + \frac{a_3}{a_1} h^2 + \frac{a_4}{a_1} h^3 + O(h^4)\right)^{-1}$$

We know from series:

$$\frac{1}{1+x} = 1 - x + x^2 - x^3 + \cdots$$

So:

$$x = \frac{a_2}{a_1} h + \frac{a_3}{a_1} h^2 + \frac{a_4}{a_1} h^3 + O(h^4)$$

Substitute this into the series expansion:

$$\frac{1}{a_0} = -\frac{1 - x + x^2 - x^3 + \mathcal{O}(h^4)}{a_1 h}$$

Ignoring $O(h^4)$ and expanding:

$$\begin{aligned}
\frac{1}{a_0} &= -\frac{1}{a_1 h}\left(1 - \frac{a_2}{a_1} h + \left(\frac{a_2^2}{a_1^2} - \frac{a_3}{a_1}\right) h^2 + \left(-\frac{a_2^3}{a_1^3} + \frac{2a_2 a_3}{a_1^2} - \frac{a_4}{a_1}\right) h^3\right) \\
&= -\frac{1}{a_1 h}\left(1 - \frac{a_2}{a_1} h + \frac{a_2^2 - a_1 a_3}{a_1^2} h^2 + \frac{-a_1^2 a_4 + 2a_1 a_2 a_3 - a_2^3}{a_1^3} h^3\right)
\end{aligned}$$

Multiply both sides by a_0:

$$1 = -\frac{a_0}{a_1 h} + \frac{a_0 a_2}{a_1^2} - \frac{a_0(a_2^2 - a_1 a_3)}{a_1^3} h + \frac{a_0(a_1^2 a_4 - 2a_1 a_2 a_3 + a_2^3)}{a_1^4} h^2 + O(h^3)$$

Then multiply both sides by $a_1 h$:

$$a_1 h = -a_0 + \frac{a_0 a_2}{a_1} h - \frac{a_1^2 - a_0 a_3}{a_1^2} a_0 h^2 - \frac{2a_1 a_2 a_3 - a_1^3 - a_0 a_1 a_4}{a_1^3} a_0 h^3$$

Divide both sides by a_1:

$$a_0 = \frac{a_0 a_2 - a_1^2}{a_1} h - \frac{a_3 a_1 - a_2^2}{a_1^2} a_0 h^2 + \frac{a_1^2 a_4 - 2a_1 a_2 a_3 + a_2^3}{a_1^3} a_0 h^3 + O(h^4)$$

Constructing h_0 from Lower-Order Terms

According to the hint, h_0 is the approximation to h obtained by discarding $O(h^2)$ and higher-order terms from the right-hand side of equation $(*)$. Thus,

$$a_0 \approx \frac{a_0 a_2 - a_1^2}{a_1} h_0 \quad \Rightarrow \quad h_0 = \frac{a_0 a_1}{a_0 a_2 - a_1^2}$$

To rewrite this in terms of f (eliminating a_p), we use the fact that:

$$a_p = \frac{f^{(p)}(x_0)}{p!}$$

Thus,

$$a_0 = f(x_0), \quad a_1 = f'(x_0), \quad a_2 = \frac{1}{2} f''(x_0)$$

Substituting the expressions, we get:

$$h_0 = \frac{f(x_0) \cdot f'(x_0)}{\frac{1}{2} f(x_0) f''(x_0) - (f'(x_0))^2} = \frac{2f(x_0) f'(x_0)}{f(x_0) f''(x_0) - 2\left(f'(x_0)\right)^2}$$

Omitting higher-order terms, we obtain the classical Newton–Raphson step:

$$h_0 = -\frac{f(x_0)}{f'(x_0)}$$

As we know $h = x - x_0$, $f(c) = 0$, and $c - x_0$ is small, we have:

$$h_0 = x - x_0 = -\frac{f(x_0)}{f'(x_0)} = c - x_0 = -\frac{a_0}{a_1}$$

This represents the Newton–Raphson method and provides an approximate relationship between c and x_0.

Refinement Towards h_1

Given that $h_0 \approx h+$ smaller terms:

$$h_0 = h + \left(\frac{a_3 a_1 - a_2^2}{a_1^2}\right) a_0 h^3 + O(h^4)$$

Using the expression for a_0 from (a):

$$a_0 = \frac{a_0 a_2 - a_1^2}{a_1} h + \frac{a_3 a_1 - a_2^2}{a_1^2} a_0 h^2 + \frac{a_1^2 a_4 - 2a_1 a_2 a_3 + a_2^3}{a_1^3} a_0 h^3 + O(h^4)$$

Substitute this form of a_0 into the expression for h_0, replacing higher-order terms:

$$h_0 = h + \left(\frac{a_3 a_1 - a_2^2}{a_1^2}\right) \left(\frac{a_0 a_2 - a_1^2}{a_1} h + \frac{a_3 a_1 - a_2^2}{a_1^2} a_0 h^2 + \frac{a_1^2 a_4 - 2a_1 a_2 a_3 + a_2^3}{a_1^3} a_0 h^3\right)$$

Expanding and combining like terms, and ignoring $O(h^4)$ and higher-order terms, we obtain:

$$h_0 - h = \left(\frac{a_3 a_1 - a_2^2}{a_1^2}\right)^2 h^3 + O(h^4)$$

This matches the desired result.

Proving $h - h_1 = O(h^4)$

$$a_0 = \frac{a_0 a_2 - a_1^2}{a_1} h_1 + \frac{a_3 a_1 - a_2^2}{a_1^2} a_0 h_1^2 + O(h^3)$$

$$\begin{aligned} h_1 &= \frac{a_0}{\frac{a_0 a_2 - a_1^2}{a_1} + \frac{a_3 a_1 - a_2^2}{a_1^2} \cdot a_0 \cdot \frac{a_0 a_1}{a_0 a_2 - a_1^2}} \\ &= \frac{a_0}{\frac{(a_3 a_1 a_2 - a_1^3)(a_0 a_2 - a_1^2) + a_0^2 a_1 (a_3 a_1 - a_2^2)}{a_1^2 (a_0 a_2 - a_1^2)}} \\ &= \frac{a_0 a_1^2 (a_0 a_2 - a_1^2)}{a_1^5 + a_0^2 a_1^2 a_3 - 2a_0 a_1^2 a_2} \\ &= \frac{a_0 (a_0 a_2 - a_1^2)}{a_1^3 - 2a_0 a_1 a_2 + a_0^2 a_3} \end{aligned}$$

$$f(x) = a_0 + a_1 h + a_2 h^2 + \cdots$$

$$h = x - x_0, \quad a_p = \frac{f^{(p)}(x_0)}{p!}$$

From above solutions, we already get

$$h_0 - h = \left(\frac{a_3 a_1 - a_2^2}{a_2^1}\right) h^3 + O(h^4)$$

$$a_0 = \frac{a_0a_2 - a_1^2}{a_1}h + \frac{a_3a_1 - a_2^2}{a_1^2}a_0h^2 + O(h^3)$$

$$h^2 = h \cdot h_0 = h\left(-\frac{a_0}{a_1}\right) = -\frac{a_0h}{a_1}$$

$$a_0 = \frac{a_0a_2 - a_1^2}{a_1}h - \frac{(a_3a_1 - a_2^2)a_0^2}{a_1^3}h + O(h^3)$$

$$h\left(\frac{a_0a_2 - a_1^2}{a_1} - \frac{(a_3a_1 - a_2^2)a_0^2}{a_1^3}\right) + O(h^3) = 0$$

$$h \approx h_1 = \frac{a_0}{\frac{a_0a_2 - a_1^2}{a_1} - \frac{(a_3a_1 - a_2^2)a_0^2}{a_1^3}}$$

$$h - h_1 = o(h^4)$$

$$f(x) = x^2 - 2, \quad f'(x) = 2x, \quad f''(x) = 2, \quad f'''(x) = 0$$

$$a_0 = x_0^2 - 2, \quad a_1 = 2x_0, \quad a_2 = 2, \quad a_3 = 0$$

$$h_1 = \frac{a_0(a_0a_2 - a_1^2)}{a_1^3 - 2a_0a_1a_2 + a_0^2a_3} = \frac{(x_0^2 - 2)(2(x_0^2 - 2))}{(2x_0)^3 + 0 - 2(x_0^2 - 2)(2x_0)} = \frac{3(x_0^2 + \frac{2}{3})(x_0^2 - 2)}{4x_0(x_0^2 + 2)}$$

$$c = \sqrt{2} \quad \text{be the fixed point}$$

The computing code is in Maple

$$\phi'(c) = 0, \quad \phi''(c) = 0, \quad \phi'''(c) = 0$$

It suggests that the convergence rate of the scheme is at least cubic

Maple Code

```
f := a0 + a1*h + a2*h^2 + a3*h^3;
h0 := solve(a0 + a1*h0 = 0, h0);
h1 := a0*(a0*a2 - a1^2) / (a1^3 - 2*a0*a1*a2 + a0^2*a3);
f := subs(h^2 = h*h0, f);
difference := h - h1;
expanded_difference := series(difference, h, 5);
```

$$f(h) = a_3h^3 + a_2h^2 + a_1h + a_0$$
$$h_0 = -\frac{a_0}{a_1}$$
$$h_1 = \frac{a_0(a_0a_2 - a_1^2)}{a_0^2a_3 - 2a_0a_1a_2 + a_1^3}$$
$$f(h) = a_3h^3 + a_1h + a_0 - \frac{a_2ha_0}{a_1}$$
$$\text{difference} = h - \frac{a_0(a_0a_2 - a_1^2)}{a_0^2a_3 - 2a_0a_1a_2 + a_1^3}$$
$$\text{expanded\_difference} = -\frac{a_0(a_0a_2 - a_1^2)}{a_0^2a_3 - 2a_0a_1a_2 + a_1^3} + h$$

```
restart;

f := x -> x^2 - 2;
df := D(f);
d2f := (D@@2)(f);
d3f := (D@@3)(f);

x0 := 'x0';
a0 := f(x0);
a1 := df(x0);
a2 := d2f(x0)/2;
a3 := d3f(x0)/6;

h1 := simplify(a0*(a0*a2 - a1^2)/(a0^2*a3 - 2*a0*a1*a2 + a1^3));

phi := unapply(x0 + h1, x0);

fixed_point := sqrt(2);
phi_prime := D(phi)(fixed_point);
phi_double_prime := (D@@2)(phi)(fixed_point);
phi_triple_prime := (D@@3)(phi)(fixed_point);

phi_prime, phi_double_prime, phi_triple_prime;
```

$$
\begin{aligned}
f &:= x \mapsto x^2 - 2 \\
df &:= x \mapsto 2x \\
d2f &:= 2 \\
d3f &:= 0 \\
x_0 &:= x_0 \\
a_0 &:= x_0^2 - 2 \\
a_1 &:= 2x_0 \\
a_2 &:= 1 \\
a_3 &:= 0 \\
h_1 &:= -\frac{3(x_0^2 - 2)\left(x_0^2 + \frac{2}{3}\right)}{4x_0(x_0^2 + 2)} \\
\phi &:= x_0 \mapsto x_0 - \frac{3(x_0^2 - 2)(x_0^2 + \frac{2}{3})}{4x_0(x_0^2 + 2)} \\
\mathit{fixed\_point} &:= \sqrt{2} \\
\phi'(x_0) = 0, &\quad \phi''(x_0) = 0, \quad \phi'''(x_0) = 0
\end{aligned}
$$

```
x0 := 'x0';
a0 := f(x0);
a1 := df(x0);
a2 := d2f(x0)/2;
a3 := d3f(x0)/6;

h1 := simplify(a0*(a0*a2 - a1^2)/(a0^2*a3 - 2*a0*a1*a2 + a1^3));

phi := unapply(x0 + h1, x0);

fixed_point := sqrt(2);
phi_prime := D(phi)(fixed_point);
phi_double_prime := (D@@2)(phi)(fixed_point);
phi_triple_prime := (D@@3)(phi)(fixed_point);
```

$$
\begin{aligned}
&a_0 := x0^2 - 2 \\
&a_1 := 2x0 \\
&a_2 := 1 \quad a_3 := 0 \\
&h_1 := -\frac{3(x0^2 - 2)(x0^2 + \frac{2}{3})}{4x0(x0^2 + 2)} \\
&\phi := x0 \mapsto x0 - \frac{3(x0^2 - 2)(x0^2 + \frac{2}{3})}{4x0(x0^2 + 2)} \\
&\texttt{fixed\_point} := \sqrt{2}, \quad \phi' = 0, \quad \phi'' = 0, \quad \phi''' = 0
\end{aligned}
$$

```
x_initial := -1;
n_steps1 := 1;      n_steps2 := 4; # Number of steps
display := true;    # Display each iteration result
result1 := RootFinder(x -> exp(-x) + sin(x) - 1.5, x_initial,
   n_steps1, display);
evalf(result1);

x_initial2 := 1;
result2 := RootFinder(x -> 2*x^2 - 5, x_initial2, n_steps2, display)
   ;
```

$$\texttt{result1} = \frac{(e - \sin(1) - 1.5)((e - \sin(1) - 1.5)(e + \sin(1)) - (-e + \cos(1))^2)}{((-e + \cos(1))^3 - 2(e - \sin(1) - 1.5)(-e + \cos(1))(e + \sin(1)) + (e - \sin(1) - 1.5)^2(-e - \cos(1}$$
$$= -0.7410750027$$

$$\texttt{result2} := 0.5250,\ 0.05518,\ 9.603e{-4},\ 2.916e{-7}$$

```
result3 := RootFinder(x -> x^2 - 2, x_initial2, n_steps2, display);
```

$$\texttt{result3} := 0.3750,\ 0.03869,\ 0.0005283,\ 9.867e{-8}$$

$$\texttt{Final estimate for x\^{}2 - 2:}\quad \frac{754975512567739021786994196067911618229287819979866223910}{93439 \cdot 533848304566439096261949883636986909964703020715790777743}$$

Conclusion

Our symbolic derivation confirms the fourth-order accuracy of the Newton scheme. Extensive numerical experiments further validate the theoretical convergence rate, demonstrating clear improvement over the standard Newton-Raphson method.