Newton's Method

MATH 375 *Numerical Analysis*

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Motivation

Newton's Method offers superior performance in root finding over the Bisection Method and *ad hoc* fixed-point methods.

We will take the approach of deriving Newton's Method using Taylor's Theorem.

Derivation

Assumptions:

- Suppose $f \in \mathcal{C}^2[a, b]$ with $f(p) = 0$ for some $p \in (a, b)$.
- Let $p_0 \in [a, b]$ with $f'(p_0) \neq 0$.

Find the linear Taylor polynomial for $f(x)$ centered at p_0.

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$$f(x) = f(p_0) + f'(p_0)(x - p_0) + \frac{f''(z(x))}{2}(x - p_0)^2$$

$$(z(x) \text{ between } x \text{ and } p_0)$$

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f(p) &= f(p_0) + f'(p_0)(p - p_0) + \frac{f''(z(p))}{2}(p - p_0)^2 \\
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&\qquad (z(p) \text{ between } p \text{ and } p_0) \\
0 &= f(p_0) + f'(p_0)\underbrace{(p - p_0)}_{\text{small}} + \frac{f''(z(p))}{2}\underbrace{(p - p_0)^2}_{\text{very small}} \\
0 &\approx f(p_0) + f'(p_0)(p - p_0) \\
p &\approx p_0 - \frac{f(p_0)}{f'(p_0)}
\end{aligned}
$$

Iterative Method

Thus if p_0 is an approximation to the root p of function f, then

$$p_1 \equiv p_0 - \frac{f(p_0)}{f'(p_0)}$$

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Thus if p_0 is an approximation to the root p of function f, then

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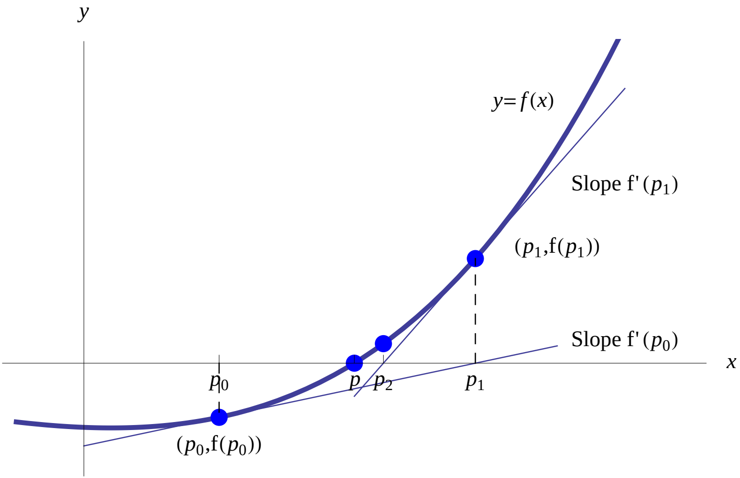
is a "better" approximation to p.

Define the sequence $\{p_n\}_{n=0}^{\infty}$ by

$$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}, \quad \text{for } n \geq 1.$$

Graphical Interpretation



Algorithm

INPUT initial approximation p_0, tolerance ϵ, maximum iterations N.

STEP 1 Set $i = 1$.

STEP 2 While $i \leq N$ do STEPS 3–6.

- STEP 3 Set $p = p_0 - \dfrac{f(p_0)}{f'(p_0)}$.
- STEP 4 If $|p - p_0| < \epsilon$ then OUTPUT p, STOP.
- STEP 5 Set $i = i + 1$.
- STEP 6 Set $p_0 = p$.

STEP 7 OUTPUT "The method failed after N iterations.", STOP.

Stopping Criteria

Remark: alternative stopping criteria may be used.

- $|p - p_0| < \epsilon$
- $\left|\frac{p - p_0}{p}\right| < \epsilon$
- $|f(p)| < \epsilon$

Stopping Criteria

Remark: alternative stopping criteria may be used.

- $|p - p_0| < \epsilon$
- $\left|\dfrac{p - p_0}{p}\right| < \epsilon$
- $|f(p)| < \epsilon$
- Since the convergence of the algorithm is not guaranteed, stopping after a maximum number of iterations can prevent “infinite loops”.

Example

Find a root of $x - 4\ln x = 0$ on interval $[1/2, 3/2]$ using $p_0 = 1$ and $\epsilon = 10^{-5}$.

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If $f(x) = x - 4\ln x$ then $f'(x) = 1 - 4/x \neq 0$ on $[1/2, 3/2]$.

$$p_n = p_{n-1} - \frac{p_{n-1} - 4\ln p_{n-1}}{1 - \frac{4}{p_{n-1}}}$$

n	p_n
0	1.00000
1	1.33333
2	1.42464
3	1.42960
4	1.42961

Convergence

Remarks:

- Newton's Method requires the initial approximation p_0 be "reasonably close" to p.
- If $f'(p_n) = 0$ for any n, the method fails.

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Theorem

If $f \in \mathcal{C}^2[a, b]$ and if $p \in (a, b)$ is such that $f(p) = 0$ and $f'(p) \neq 0$, then there exists $\delta > 0$ such that Newton's Method generates a sequence $\{p_n\}_{n=0}^{\infty}$ converging to p for any initial approximation $p_0 \in [p - \delta, p + \delta]$.

Proof (1 of 3)

- Let $g(x) = x - \dfrac{f(x)}{f'(x)}$, then $p_n = g(p_{n-1})$.
- Choose $k \in (0, 1)$.

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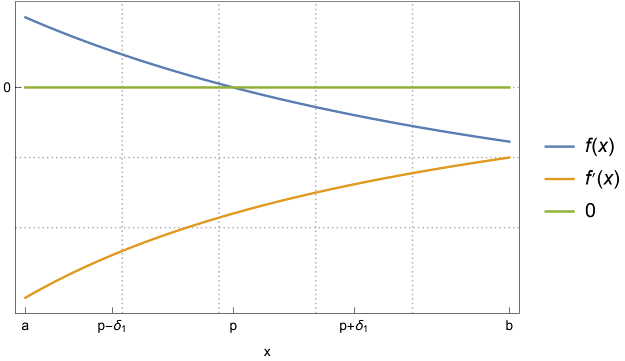
- Choose $k \in (0, 1)$.
- Since f' is continuous and $f'(p) \neq 0$, then there exists $\delta_1 > 0$ such that $f'(x) \neq 0$ for all $x \in [p - \delta_1, p + \delta_1] \subseteq [a, b]$. Consequently $g(x)$ is defined and continuous for all $x \in [p - \delta_1, p + \delta_1]$.

Illustration

$$g(x) = x - \frac{f(x)}{f'(x)}$$



Function $g(x)$ is defined and continuous for all $x \in [p - \delta_1, p + \delta_1]$.

Proof (2 of 3)

$$
\begin{aligned}
g(x) &= x - \frac{f(x)}{f'(x)} \\
g'(x) &= 1 - \frac{f'(x)\,f'(x) - f(x)\,f''(x)}{[f'(x)]^2} \\
&= \frac{f(x)\,f''(x)}{[f'(x)]^2}
\end{aligned}
$$

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Since $f \in \mathcal{C}^2[a, b]$ then $g \in \mathcal{C}^1[p - \delta_1, p + \delta_1]$.

$$g'(p) = \frac{f(p)\, f''(p)}{[f'(p)]^2} = 0$$

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Since $f \in \mathcal{C}^2[a, b]$ then $g \in \mathcal{C}^1[p - \delta_1, p + \delta_1]$.

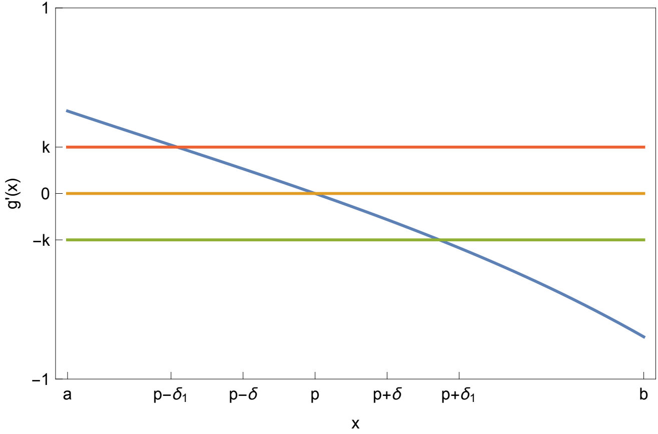
$$g'(p) = \frac{f(p)\,f''(p)}{[f'(p)]^2} = 0$$

Since g' is continuous there exists $0 < \delta < \delta_1$ such that

$$|g'(x)| \leq k < 1, \quad \text{for all } [p - \delta, p + \delta].$$

Illustration

$$g'(x) = \frac{f(x)f''(x)}{(f'(x))^2}$$



$$|g'(x)| \leq k < 1, \quad \text{for all } [p-\delta, p+\delta].$$

Proof (3 of 3)

- Suppose $x \in [p-\delta, p+\delta]$, by the MVT there is a z between x and p such that

$$\begin{aligned}
\left|\frac{g(x)-g(p)}{x-p}\right| &= |g'(z)| \\
|g(x)-g(p)| &= |g'(z)|\,|x-p| \\
|g(x)-p| &\leq k|x-p| \\
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- Since $|x-p| < \delta$ then $|g(x)-p| < \delta$, *i.e.*, function g maps the interval $[p-\delta, p+\delta]$ into itself.

Proof (3 of 3)

- Suppose $x \in [p - \delta, p + \delta]$, by the MVT there is a z between x and p such that

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\left| \frac{g(x) - g(p)}{x - p} \right| &= |g'(z)| \\
|g(x) - g(p)| &= |g'(z)|\,|x - p| \\
|g(x) - p| &\leq k|x - p| \\
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- Since $|x - p| < \delta$ then $|g(x) - p| < \delta$, *i.e.*, function g maps the interval $[p - \delta, p + \delta]$ into itself.
- By the Fixed-Point Theorem applied to g, the sequence $\{p_n\}_{n=0}^{\infty}$ converges to the unique fixed point p.

General Comments

1. Convergence of the algorithm is not guaranteed.
2. Good initial approximation of the root is often needed for convergence.
3. Must evaluate $f(x)$ and $f'(x)$ on each iteration.
4. If the root at $x = p$ is not a simple root (*e.g.*, if $f'(p) = 0$), the convergence can be slow.
5. Since $\dfrac{d}{dx}\left[x - \dfrac{f(x)}{f'(x)}\right]_{x=p} = \dfrac{f(p)f''(p)}{(f'(p))^2} = 0$, Newton's method converges quadratically.

Multiple Root Issue

Let $f(x) = x^2$ and $g(x) = x^3$ and $p_0 = 0.5$.

n	$p_{n-1} - \dfrac{f(p_{n-1})}{f'(p_{n-1})}$	$p_{n-1} - \dfrac{g(p_{n-1})}{g'(p_{n-1})}$
1	0.25000	0.33333
2	0.12500	0.22222
3	0.06250	0.14815
4	0.03125	0.09877
5	0.01563	0.06584
6	0.00781	0.04390
7	0.00391	0.02926

Avoiding the Derivative

One drawback of Newton's Method is the need to evaluate the derivative $f'(p_{n-1})$ in addition to evaluating $f(p_{n-1})$.

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\begin{aligned}
f'(p_{n-1}) &= \lim_{x \to p_{n-1}} \frac{f(x) - f(p_{n-1})}{x - p_{n-1}} \\
&\approx \frac{f(p_{n-2}) - f(p_{n-1})}{p_{n-2} - p_{n-1}} \\
&= \frac{f(p_{n-1}) - f(p_{n-2})}{p_{n-1} - p_{n-2}}
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Substitute into the Newton's Method Formula to obtain

$$p_n = p_{n-1} - \frac{f(p_{n-1})(p_{n-1} - p_{n-2})}{f(p_{n-1}) - f(p_{n-2})}$$

known as the **Secant Method**.

Algorithm: Secant Method

INPUT initial approximations p_0, p_1, tolerance ϵ, maximum iterations N.

STEP 1 Set $i = 2$; $q_0 = f(p_0)$; $q_1 = f(p_1)$.

STEP 2 While $i \leq N$ do STEPS 3–6.

STEP 3 Set $p = p_1 - \dfrac{q_1(p_1 - p_0)}{q_1 - q_0}$.

STEP 4 If $|p - p_1| < \epsilon$ then OUTPUT p, STOP.

STEP 5 Set $i = i + 1$.

STEP 6 Set $p_0 = p_1$; $q_0 = q_1$; $p_1 = p$; $q_1 = f(p)$.

STEP 7 OUTPUT "The method failed after N iterations.", STOP.

Example

Use the Secant Method to approximate a solution to $x - 4\ln x = 0$ using $p_0 = 1$ and $p_1 = 1.5$.

Secant

n	p_n
0	1.00000
1	1.50000
2	1.44569
3	1.42962
4	1.42961

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Newton

n	p_n
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  This is not true of Newton's Method or the Secant Method.
- The Secant Method can be modified to bracket the root.

Algorithm: False Position

INPUT initial approximations p_0, p_1, tolerance ϵ, maximum iterations N.

STEP 1 Set $i = 2$; $q_0 = f(p_0)$; $q_1 = f(p_1)$.

STEP 2 While $i \leq N$ do STEPS 3–7.

- STEP 3 Set $p = p_1 - \dfrac{q_1(p_1 - p_0)}{q_1 - q_0}$.
- STEP 4 If $|p - p_1| < \epsilon$ then OUTPUT p, STOP.
- STEP 5 Set $i = i + 1$; $q = f(p)$.
- STEP 6 If $q \cdot q_1 < 0$ set $p_0 = p_1$; $q_0 = q_1$.
- STEP 7 Set $p_1 = p$; $q_1 = q$.

STEP 8 OUTPUT "The method failed after N iterations.", STOP.

Example

Use the Method of False Position approximate a solution to $x - 4 \ln x = 0$ using $p_0 = 1$ and $p_1 = 1.5$.

False Position

n	p_n
0	1.00000
1	1.50000
2	1.44569
3	1.43327
4	1.43045
5	1.42980
6	1.42965
7	1.42962
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Uniqueness of Order of Convergence

Lemma

The order of convergence of a sequence is unique.

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Proof.

Suppose $\lim_{n\to\infty} \alpha_n = \alpha$ and there exist $0 < p < q$ and positive constants λ and μ such that

$$\lim_{n\to\infty} \frac{|\alpha_{n+1} - \alpha|}{|\alpha_n - \alpha|^p} = \lambda \text{ and } \lim_{n\to\infty} \frac{|\alpha_{n+1} - \alpha|}{|\alpha_n - \alpha|^q} = \mu.$$

Consider the limit

$$\begin{aligned}
\lim_{n\to\infty} \frac{|\alpha_{n+1} - \alpha|}{|\alpha_n - \alpha|^p} &= \lim_{n\to\infty} \frac{|\alpha_{n+1} - \alpha|}{|\alpha_n - \alpha|^q |\alpha_n - \alpha|^{p-q}} \\
&= \lim_{n\to\infty} \frac{|\alpha_{n+1} - \alpha|}{|\alpha_n - \alpha|^q} \lim_{n\to\infty} \frac{1}{|\alpha_n - \alpha|^{p-q}} \\
&= \mu \lim_{n\to\infty} |\alpha_n - \alpha|^{q-p} \\
&= \mu(0) = 0,
\end{aligned}$$

a contradiction.

Rate of Convergence of Secant Method (1 of 5)

Suppose p is a root of the equation $f(x) = 0$ and $f'(p) \neq 0 \neq f''(p)$ and $f'''(x)$ exists in an open interval containing p.

$$\text{Secant method: } x_{n+1} = x_n - \frac{f(x_n)(x_n - x_{n-1})}{f(x_n) - f(x_{n-1})}$$

Let $\{x_n\}_{n=0}^{\infty}$ be the sequence generated by the Secant method where $\lim_{n\to\infty} x_n = p$. Define $e_n = x_n - p$.

$$\begin{aligned} x_{n+1} &= e_{n+1} + p = e_n + p - \frac{f(p+e_n)(p+e_n-p-e_{n-1})}{f(p+e_n) - f(p+e_{n-1})} \\ e_{n+1} &= e_n - \frac{f(p+e_n)(e_n - e_{n-1})}{f(p+e_n) - f(p+e_{n-1})} \end{aligned}$$

Expand $f(x)$ as a Taylor polynomial about p.

$$f(x) = f(p) + f'(p)(x-p) + \frac{f''(p)}{2}(x-p)^2 + \frac{f'''(z)}{6}(x-p)^3$$

Rate of Convergence of Secant Method (2 of 5)

Replace f by its Taylor polynomial expansion.

$$
\begin{aligned}
e_{n+1} &= e_n - \frac{f(p+e_n)(e_n - e_{n-1})}{f(p+e_n) - f(p+e_{n-1})} \\
&= e_n - (e_n - e_{n-1}) \frac{f'(p)e_n + \frac{f''(p)}{2}e_n^2 + O(e_n^3)}{f'(p)e_n + \frac{f''(p)}{2}e_n^2 + O(e_n^3) - f'(p)e_{n-1} - \frac{f''(p)}{2}e_{n-1}^2 - O(e_{n-1}^3)} \\
&= e_n - (e_n - e_{n-1}) \frac{e_n + \frac{f''(p)}{2f'(p)}e_n^2 + O(e_n^3)}{e_n + \frac{f''(p)}{2f'(p)}e_n^2 + O(e_n^3) - e_{n-1} - \frac{f''(p)}{2f'(p)}e_{n-1}^2 - O(e_{n-1}^3)} \\
&= e_n - (e_n - e_{n-1}) \frac{e_n + \frac{f''(p)}{2f'(p)}e_n^2 + O(e_n^3)}{(e_n - e_{n-1}) + \frac{f''(p)}{2f'(p)}(e_n^2 - e_{n-1}^2) + O(e_n^3) - O(e_{n-1}^3)} \\
&= e_n - \frac{e_n + \frac{f''(p)}{2f'(p)}e_n^2 + O(e_n^3)}{1 + (e_n + e_{n-1})\frac{f''(p)}{2f'(p)} + \frac{O(e_n^3) - O(e_{n-1}^3)}{e_n - e_{n-1}}}
\end{aligned}
$$

Since $e_k \to 0$ as $k \to \infty$ the expression $O(e_{n-1}^3)$ dominates $O(e_n^3)$.

Rate of Convergence of Secant Method (3 of 5)

$$
\begin{aligned}
e_{n+1} &= e_n - \frac{e_n + \frac{f''(p)}{2f'(p)} e_n^2 + O(e_n^3)}{1 + (e_n + e_{n-1})\frac{f''(p)}{2f'(p)} - \frac{O(e_{n-1}^3)}{e_n - e_{n-1}}} \\
&= \frac{e_n \left(1 + (e_n + e_{n-1})\frac{f''(p)}{2f'(p)} - \frac{O(e_{n-1}^3)}{e_n - e_{n-1}}\right) - e_n - \frac{f''(p)}{2f'(p)} e_n^2 - O(e_n^3)}{1 + (e_n + e_{n-1})\frac{f''(p)}{2f'(p)} - \frac{O(e_{n-1}^3)}{e_n - e_{n-1}}} \\
&= \frac{e_n e_{n-1}\frac{f''(p)}{2f'(p)} - O(e_{n-1}^3)\frac{e_n}{e_n - e_{n-1}} - O(e_n^3)}{1 + (e_n + e_{n-1})\frac{f''(p)}{2f'(p)} - \frac{O(e_{n-1}^3)}{e_n - e_{n-1}}}
\end{aligned}
$$

Suppose the order of convergence of $\{x_n\}_{n=0}^{\infty}$ is α, then

$$
\lim_{n\to\infty} \frac{|p - x_{n+1}|}{|p - x_n|^{\alpha}} = \lim_{n\to\infty} \frac{|e_{n+1}|}{|e_n|^{\alpha}} = \lambda \neq 0.
$$

Rate of Convergence of Secant Method (4 of 5)

$$\begin{aligned}
\lim_{n\to\infty} \frac{|e_{n+1}|}{|e_n|^\alpha} &= \lim_{n\to\infty} \left| \frac{e_n^{1-\alpha} e_{n-1} \frac{f''(p)}{2f'(p)} - O(e_{n-1}^3) \frac{e_n^{1-\alpha}}{e_n - e_{n-1}} - O(e_n^{3-\alpha})}{1 + (e_n + e_{n-1}) \frac{f''(p)}{2f'(p)} - \frac{O(e_{n-1}^3)}{e_n - e_{n-1}}} \right| \\
&= \lambda \neq 0
\end{aligned}$$

Since $\lim_{n\to\infty} e_n = \lim_{n\to\infty} e_{n-1} = 0$ then it must be the case that $\lim_{n\to\infty} |e_n^{1-\alpha} e_{n-1}|$ converges to a positive value, say $C > 0$.

$$\begin{aligned}
C &= \lim_{n\to\infty} |e_n^{1-\alpha} e_{n-1}| \\
C &= \lim_{n\to\infty} |e_{n+1}^{1-\alpha} e_n| \\
C^{\frac{1}{1-\alpha}} &= \lim_{n\to\infty} \left| e_{n+1} e_n^{\frac{1}{1-\alpha}} \right| \\
C^{\frac{1}{1-\alpha}} &= \lim_{n\to\infty} \frac{|e_{n+1}|}{|e_n|^{1/(\alpha-1)}}
\end{aligned}$$

which implies the rate of convergence is $O(e_n^{1/(\alpha-1)})$.

Rate of Convergence of Secant Method (5 of 5)

Since the rate of convergence of a sequence is unique then,

$$\begin{aligned} \alpha &= \frac{1}{\alpha - 1} \\ \alpha^2 - \alpha - 1 &= 0 \\ \alpha &= \frac{1 + \sqrt{5}}{2} \\ &\approx 1.61803. \end{aligned}$$

Homework

- Read Section 2.3.
- Exercises: 5, 7, 17, 19, 23, 27