Solutions of Non-linear Equations

in One Variable

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1. linear if \exists a constant 0 < c < 1 and an integer N > 0 such that

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2. superlinear if $\exists \{c_n\}, c_n \to 0$ as $n \to \infty$, and an integer N > 0 such that

$$|x_{n+1} - x^*| \le c_n |x_n - x^*|, \quad \forall \ n \ge N,$$

or, equivalently,

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3. quadratic if \exists a constant c > 0 (not necessarily less than 1) and an integer N > 0 such that

$$|x_{n+1} - x^*| \le c|x_n - x^*|^2, \quad \forall \ n \ge N.$$

In general, if there are positive constants c and α and an integer N > 0 such that

$$|x_{n+1} - x^*| \le c |x_n - x^*|^{\alpha}, \quad \forall \ n \ge N,$$

then we say the rate of convergence is of order α .

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Definition 2 Suppose $\{\beta_n\} \to 0$ and $\{x_n\} \to x^*$. If $\exists c > 0$ and an integer N > 0 such that

$$|x_n - x^*| \le c|\beta_n|, \quad \forall \ n \ge N,$$

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Example 1 Compare the convergence behavior of $\{x_n\}$ and $\{y_n\}$, where

$$x_n = \frac{n+1}{n^2}$$
, and $y_n = \frac{n+3}{n^3}$.

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Let $\alpha_n = \frac{1}{n}$ and $\beta_n = \frac{1}{n^2}$. Then

$$\begin{aligned} |x_n - 0| &= \frac{n+1}{n^2} \le \frac{n+n}{n^2} = \frac{2}{n} = 2\alpha_n, \\ |y_n - 0| &= \frac{n+3}{n^3} \le \frac{n+3n}{n^3} = \frac{4}{n^2} = 4\beta_n. \end{aligned}$$

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Hence

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This shows that $\{y_n\}$ converges to 0 much faster than $\{x_n\}$.

2 – Bisection Method

Idea: if $f(x) \in C[a, b]$ and f(a)f(b) < 0, then $\exists c \in (a, b)$ such that f(c) = 0.

Algorithm 1 (Bisection Method) Given f(x) defined on (a, b), the maximal number of iterations M, and stop criteria δ and ε , this algorithm tries to locate one root of f(x).

compute
$$u = f(a)$$
, $v = f(b)$, and $e = b - a$.
if $sign(u) = sign(v)$, then stop
for $k = 1, 2, ..., M$ do
 $e = e/2, c = a + e, w = f(c)$.
if $|e| < \delta$ or $|w| < \varepsilon$, then stop
if $sign(w) \neq sign(u)$ then
 $b = c, v = w$.
else
 $a = c, u = w$
end if
end for

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- 1. the iteration number k > M,
- 2. $|c_k c_{k-1}| < \delta$, or
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 $\Rightarrow \{a_n\}$ and $\{b_n\}$ are bounded.

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 $\Rightarrow \{a_n\} \text{ and } \{b_n\} \text{ are bounded.}$ $\Rightarrow \lim_{n \to \infty} a_n \text{ and } \lim_{n \to \infty} b_n \text{ exist.}$

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Since
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 $\Rightarrow \lim_{n \to \infty} f(a_n)f(b_n) = f^2(z) \leq 0$.
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$$\Rightarrow \text{ The limit of the sequences } \{a_n\} \text{ and } \{b_n\} \text{ is a zero of } f \text{ in } [a, b].$$
Let $c_n = \frac{1}{2}(a_n + b_n).$ Then
$$|z - c_n| = |\lim_{n \to \infty} a_n - \frac{1}{2}(a_n + b_n)|$$

$$= |\frac{1}{2} [\lim_{n \to \infty} a_n - b_n] + \frac{1}{2} [\lim_{n \to \infty} a_n - a_n] |$$

$$\leq \frac{1}{2} \max \{|\lim_{n \to \infty} a_n - b_n|, |\lim_{n \to \infty} a_n - a_n|\}$$

$$\leq \frac{1}{2} |b_n - a_n| = \frac{1}{2^{n+1}} |b_0 - a_0|.$$

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Since $f(a_n)f(b_n) \le 0$. $\Rightarrow \lim_{n \to \infty} f(a_n) f(b_n) = f^2(z) \le 0.$ $\Rightarrow f(z) = 0.$ \Rightarrow The limit of the sequences $\{a_n\}$ and $\{b_n\}$ is a zero of f in [a, b]. Let $c_n = \frac{1}{2}(a_n + b_n)$. Then $|z - c_n| = \left| \lim_{n \to \infty} a_n - \frac{1}{2}(a_n + b_n) \right|$ $= \left|\frac{1}{2}\left[\lim_{n \to \infty} a_n - b_n\right] + \frac{1}{2}\left[\lim_{n \to \infty} a_n - a_n\right]\right|$ $\leq \frac{1}{2} \max\left\{ \left| \lim_{n \to \infty} a_n - b_n \right|, \left| \lim_{n \to \infty} a_n - a_n \right| \right\}$ $\leq \frac{1}{2}|b_n - a_n| = \frac{1}{2^{n+1}}|b_0 - a_0|.$ This proves the following theorem.

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Theorem 1 Let $\{[a_n, b_n]\}$ denote the intervals produced by the bisection algorithm. Then $\lim_{n \to \infty} a_n$ and $\lim_{n \to \infty} b_n$ exist, are equal, and represent a zero of f(x). If



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 $z = \lim_{n \to \infty} a_n = \lim_{n \to \infty} b_n$ and $c_n = \frac{1}{2}(a_n + b_n)$, then $|z - c_n| \le \frac{1}{2^{n+1}} (b_0 - a_0).$ **Remarks 1** $\{c_n\}$ converges to z with the rate of $O(2^{-n})$.

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Remarks 1 $\{c_n\}$ converges to z with the rate of $O(2^{-n})$.

Example 2 If bisection method starts with interval [50, 75], then how many steps should be taken to compute a root with relative error that is less than 10^{-12} ?

 $|z - c_n| \le \frac{1}{2^{n+1}} (b_0 - a_0).$

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then



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Solution: Seek an n such that

$$\frac{|z - c_n|}{|z|} \le 10^{-12}.$$

Since the bisection method starts with the interval [50, 75], this implies that $z \ge 50$, hence it is sufficient to show

$$\frac{|z - c_n|}{|z|} \le \frac{|z - c_n|}{50} \le 10^{-12}.$$

That is, we solve

$$2^{-(n+1)}(75-50) \le 50 \times 10^{-12}$$

for n, which gives $n \ge 38$.

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3.1 – Derivation of Newton's Method

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$$0 = f(x^*) = f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{3!}f'''(x)h^3 + \cdots$$
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Since *h* is small, $O(h^2)$ is negligible. It is reasonable to drop $O(h^2)$ terms. This implies

$$f(x) + f'(x)h \approx 0$$
 and $h \approx -\frac{f(x)}{f'(x)}$, if $f'(x) \neq 0$.

Hence

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Figure 1: Newton-Rapbson method

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$$f(x) = f(x_k) + f'(x_k)(x - x_k) + \frac{1}{2}f''(x_k)(x - x_k)^2 + \cdots$$

Figure 3 gives a graphic interpretation of the Newton's method. Since the Taylor's expansion of f(x) at x_k is given by

$$f(x) = f(x_k) + f'(x_k)(x - x_k) + \frac{1}{2}f''(x_k)(x - x_k)^2 + \cdots$$

At x_k , one uses the tangent line

$$y = \ell(x) = f(x_k) + f'(x_k)(x - x_k)$$

to approximate the curve of f(x) and uses the zero of the tangent line to approximate the zero of f(x).

Algorithm 2 (Newton's Method) Given a function $f : \mathbb{R} \to \mathbb{R}$, an initial guess x_0 to the zero of f, and stop criteria M, δ , and ε , this algorithm performs the Newton's iteration to approximate one root of f.

$$\begin{split} & u = f(x_0) \\ & v = f'(x_0) \\ & x_1 = x_0 - \frac{u}{v} \\ & k = 1 \\ & u = f(x_k) \\ & \text{while } (k < M) \text{ and } (|x_k - x_{k-1}| \ge \delta) \text{ and } (|f(x_k)| \ge \varepsilon \text{ do} \\ & v = f'(x_k) \\ & x_{k+1} = x_k - \frac{u}{v} \\ & k = k+1 \\ & u = f(x_k) \\ \end{split}$$

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$$D = \{x; |x - x^*| \le \delta\}$$

and

$$\gamma = \frac{1}{2} \cdot \frac{\max_{x \in D} |f''(x)|}{\min_{x \in D} |f'(x)|}$$

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$$0 = f(x^*) = f(x_0) + f'(x_0)(x^* - x_0) + \frac{1}{2}f''(\xi_0)(x^* - x_0)^2,$$

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Choose δ such that $\rho = \delta \gamma < 1$. Suppose $|e_0| = |x_0 - x^*| \le \delta$. By Taylor's theorem

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where ξ_0 is between x^* and x_0 . Consequently $|\xi_0 - x^*| \leq \delta$ and

$$-f(x_0) - f'(x_0)(x^* - x_0) = \frac{1}{2}f''(\xi_0)(x^* - x_0)^2.$$

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$$e_{1} = x_{1} - x^{*} = x_{0} - \frac{f(x_{0})}{f'(x_{0})} - x^{*}$$

$$= \frac{1}{f'(x_{0})} \left(-f(x_{0}) - f'(x_{0})(x^{*} - x_{0})\right)$$

$$= \frac{1}{f'(x_{0})} \cdot \frac{1}{2} \cdot f''(\xi_{0})(x^{*} - x_{0})^{2} = \frac{f''(\xi_{0})}{2f'(x_{0})}e_{0}^{2},$$

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$$|e_1| \le \gamma |e_0|^2 \le \gamma \delta |e_0| = \rho |e_0|.$$

In general,

$$|e_k| \le \rho |e_{k-1}| \le \dots \le \rho^k |e_0|$$

Since $\rho < 1$, $|e_k| \to 0$ as $k \to 0$, that is, $x_k \to x^*$.

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To investigate the convergence rate, we start with

$$e_{k+1} = x_{k+1} - x^* = x_k - \frac{f(x_k)}{f'(x_k)} - x^* = \frac{f'(x_k)e_k - f(x_k)}{f'(x_k)}$$

In summary, Newton's method will generate $\{x_k\}_{k\geq 0}$ that converges to the zero, x^* , of f if

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Hence

$$|e_{k+1}| = \frac{|f''(\xi_k)|}{2|f'(x_k)|} |e_k|^2 \approx \frac{|f''(x^*)|}{2|f'(x^*)|} |e_k|^2 \equiv C|e_k|^2.$$

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Theorem 2 Assume $f(x^*) = 0$, $f'(x^*) \neq 0$ and f(x), f'(x) and f''(x) are continuous on $N_{\varepsilon}(x^*)$. Then if x_0 is chosen sufficiently close to x^* , then

$$\left\{x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}\right\} \to x^*.$$

Moreover,

$$\lim_{n \to \infty} \frac{x^* - x_{n+1}}{(x^* - x_n)^2} = -\frac{f''(x^*)}{2f'(x^*)}$$
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Definition 3 (Lipschitz Continuous) A function f(x) is Lipschitz continuous with Lipschitz constant γ in a set X, written $f \in \mathcal{L}ip_{\gamma}(X)$, if

$$|f(x) - f(y)| \le \gamma |x - y|, \text{ for all } x, y \in X.$$

Lemma 1 Suppose $f : \Omega \to \mathbb{R}$ for some open interval $\Omega \subseteq \mathbb{R}$ and $f' \in \mathcal{L}ip_{\gamma}(\Omega)$. Then for all $x, y \in \Omega$,

$$|f(y) - f(x) - f'(x)(y - x)| \le \frac{\gamma}{2}(y - x)^2.$$

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By changing variable u=x+t(y-x), $du=(y-x)\,dt$ and $f'\in\mathcal{L}\textit{ip}_{\gamma}(\Omega),$ we have

$$\begin{aligned} |f(y) - f(x) - f'(x)(y - x)| &= \left| \int_0^1 \left[f'(x + t(y - x)) - f'(x) \right](y - x) \, dt \right| \\ &\leq |y - x| \int_0^1 \gamma |t(y - x)| \, dt \\ &= \frac{\gamma}{2} |y - x|^2. \end{aligned}$$

Theorem 3 Let $f: \Omega \to \mathbb{R}$ for some open interval $\Omega \subseteq \mathbb{R}$. Assume

- 1. $\exists x^* \in \Omega$ such that $f(x^*) = 0$;
- 2. $f' \in \mathcal{L}ip_{\gamma}(\Omega);$
- 3. $\exists \rho > 0$ such that $|f'(x)| \ge \rho \ \forall x \in \Omega$, that is, $f'(x) \ne 0 \ \forall x \in \Omega$.

Then $\exists \eta > 0$ such that if $|x_0 - x^*| < \eta$, then

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, \quad k = 0, 1, 2, \dots,$$

converges to x^* . Furthermore,

$$|x_{k+1} - x^*| \le \frac{\gamma}{2\rho} |x_k - x^*|^2$$

or, equivalently,

$$|e_{k+1}| \le \frac{\gamma}{2\rho} |e_k|^2.$$

Proof: With the result of previous Lemma,

$$\begin{aligned} x_{k+1} - x^* | &= \left| x_k - \frac{f(x_k)}{f'(x_k)} - x^* \right| \\ &= \left| x_k - x^* - \frac{f(x_k) - f(x^*)}{f'(x_k)} \right| \\ &= \frac{1}{|f'(x_k)|} |f(x^*) - f(x_k) - f'(x_k)(x_k - x^*)| \\ &\leq \frac{\gamma}{2|f'(x_k)|} |x_k - x^*|^2 \\ &\leq \frac{\gamma}{2\rho} |x_k - x^*|^2. \end{aligned}$$

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(i) Newton's method only guarantee the convergence from a good starting point x_0 that is close enough to x^* . In fact, Newton's iteration may not converge at all if $|x_0 - x^*|$ is large.

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- (ii) If $f'(x^*) = 0$, i.e., x^* is a multiple root of f, then Newton's method converges only linearly.
- (iii) When f is a linear function, Newton's method will converge in one step.

Example 3 The following table shows the convergence behavior of Newton's method applied to solving $f(x) = x^2 - 1 = 0$. Observe the quadratic convergence rate.

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k	x_k	$ e_k $
0	2.0	1
1	1.25	0.25
2	1.025	2.5e-2
3	1.0003048780488	3.048780488e-4
4	1.0000000464611	4.64611e-8
5	1.0	0

Example 4 Newton's method will fail (the sequence $\{x_k\}$ does not converge) on solving $f(x) = x^2 - 4x + 5 = 0$ since f does not have any real root.

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Example 5 When Newton's method applied to $f(x) = \cos x$ with starting point $x_0 = 3$, which is close to the root $\frac{\pi}{2}$ of f, it produces $x_1 = -4.01525, x_2 = -4.8526, \cdots$, which converges to another root $-\frac{3\pi}{2}$.



Figure 2: one step of Newton method

Example 6 When Newton's method applied to $f(x) = x^3 - x - 3$ with starting point $x_0 = 0$, it produces

$x_1 = -3$	$x_2 = -1.961538$
$x_3 = -1.147176$	$x_4 = -0.00679$
$x_5 = -3.000389$	$x_6 = -1.961818$
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The sequence converges to the root 1.671699881. This example illustrates that the starting point x_0 must be close enough to the zero of f.

4 – Quasi-Newton's Method (Secant Method)

4.1 – The Secant Method

Newton's iteration:

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

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Since

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h},$$

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Since

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h},$$

 \Rightarrow

$$f'(x_k) \approx \frac{f(x_k + h_k) - f(x_k)}{h_k}$$
 for some small h_k .

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 \Rightarrow The finite-difference Newton's iteration

$$x_{k+1} = x_k - f(x_k) \frac{h_k}{f(x_k + h_k) - f(x_k)}$$

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Figure 3: Secant method

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The slope of the secant line is

$$s_k = \frac{f(x_k + h_k) - f(x_k)}{h_k}$$

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Set

$$h_k = x_k - x_{k-1}.$$

This leads to the so-called secant method or quasi-Newton method.

$$x_{k+1} = x_k - f(x_k) \frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})}.$$

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Note that the secant method requires two initial guesses x_0 and x_{-1} .

Example 7 The following table shows the convergence history for the finite-difference Newton's method with $h_k = 10^{-7} \times x_k$ and secant method for solving $f(x) = x^2 - 1 = 0.$

	finite-difference Newton	secant method
x_0	2	2
x_1	1.2500000266453	1.2500000266453
x_2	1.0250000179057	1.0769230844910
x_3	1.0003048001120	1.0082644643823
x_4	1.0000000464701	1.0003048781354
x_5	1	1.0000012544523
x_6		1.0000000001912
x_7		1

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4.2 – Error Analysis of Secant Method

Let x^* denote the exact solution of f(x) = 0, $e_k = x_k - x^*$ be the errors at the k-th step. Then

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= $x_k - f(x_k) \frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})} - x^*$
= $\frac{1}{f(x_k) - f(x_{k-1})} [(x_{k+1} - x^*)f(x_k) - (x_k - x^*)f(x_{k-1})]$

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$$= \frac{1}{f(x_k) - f(x_{k-1})} (e_{k-1}f(x_k) - e_k f(x_{k-1}))$$

$$= e_k e_{k-1} \left(\frac{\frac{1}{e_k}f(x_k) - \frac{1}{e_{k-1}}f(x_k)}{x_k - x_{k-1}} \cdot \frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})} \right)$$

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To estimate the numerator -

$$r \frac{\frac{1}{e_k} f(x_k) - \frac{1}{e_{k-1}} f(x_k)}{x_k - x_{k-1}},$$

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To estimate the numerator $\frac{\frac{1}{e_k}f(x_k) - \frac{1}{e_{k-1}}f(x_k)}{x_k - x_{k-1}}$, we apply the Taylor's theorem

$$f(x_k) = f(x^* + e_k) = f(x^*) + f'(x^*)e_k + \frac{1}{2}f''(x^*)e_k^2 + O(e_k^3),$$

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Similarly,

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Hence

$$\frac{1}{e_k}f(x_k) - \frac{1}{e_{k-1}}f(x_{k-1}) \approx \frac{1}{2}(e_k - e_{k-1})f''(x^*).$$

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Since $x_k - x_{k-1} = e_k - e_{k-1}$ and

$$\frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})} \to \frac{1}{f'(x^*)},$$

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Remark 2 Two steps of secant method would require a little more work than one step of Newton's method.



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Two questions arise: "When does a function have a fixed point?" and "How to find a fixed point?".

5.1 – Functional Iteration

Fixed-point iteration or functional iteration: Given a continuous function f,

choose an initial point x_0 and generate $\{x_k\}_{k\geq 0}$ by

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Note that Newton's method for solving g(x) = 0

$$x_{k+1} = x_k - \frac{g(x_k)}{g'(x_k)}$$

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is just a special case of functional iteration in which

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Definition 5 A function (mapping) f is said to be contractive if there exists a constant $0 \le \lambda < 1$ such that

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Theorem 4 (Contractive Mapping Theorem) Suppose $f : D \to D$, where $D \subseteq \mathbb{R}$ is a closed set, is a contractive mapping. Then f has a unique fixed point in D. Moreover, this fixed point is the limit of every sequence obtained by

$$x_{k+1} = f(x_k)$$

with any initial point x_0 .



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Since f is contractive, we have

$$\begin{aligned} x_{i} - x_{i-1} &= |f(x_{i-1}) - f(x_{i-2})| \\ &\leq \lambda |x_{i-1} - x_{i-2}| \\ &\leq \lambda^{2} |x_{i-2} - x_{i-3}| \\ &\vdots \\ &\leq \lambda^{i-1} |x_{1} - x_{0}|. \end{aligned}$$

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$$\Rightarrow x^* = \lim_{k \to \infty} x_k = \lim_{k \to \infty} f(x_{k-1}) = f(\lim_{k \to \infty} x_{k-1}) = f(x^*)$$

$$\Rightarrow x^* \text{ is a fixed point of } f.$$

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Theorem 5 If $f \in C[a, b]$ such that $a \leq f(x) \leq b$ for all $x \in [a, b]$, then f has a fixed point in [a, b]. Suppose, in addition, that f'(x) exists in (a, b) and there exists a positive constant M < 1 such that $|f'(x)| \leq M < 1$ for all $x \in (a, b)$. Then the fixed point is unique.

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Proof: If f(a) = a or f(b) = b, then a or b is a fixed point of f and we are done. Otherwise, it must be g(a) > a and g(b) < b. Let h(x) = f(x) - x. $\Rightarrow h \in C[a, b]$ since $f \in C[a, b]$, and h(a) = f(a) - a > 0, h(b) = f(b) - b < 0.
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However, this contradicts to the assumption that $f'(x) \le M < 1$ for all x in [a, b]. Therefore the fixed point of f is unique.

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5.2 – Convergence Analysis

Assumptions:

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1. f has a fixed point x^* , and the sequence $\{x_k\}_{k\geq 0}$ is generated by the iteration

$$x_{k+1} = f(x_k), \quad k = 0, 1, \dots,$$

with an arbitrary initial point x_0 ;

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$$e_{k+1} = x_{k+1} - x^* = f(x_k) - f(x^*) = f'(\xi_k)(x_k - x^*) = f'(\xi_k)e_k$$
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= $f'(x^*)e_k + \frac{1}{2}f''(x^*)e_k^2 + \dots + \frac{1}{(m-1)!}f^{(m-1)}(x^*)e_k^{m-1}$
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Therefore we have

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This shows that the convergence rate of the functional iteration is m.

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