Chapter Two. Iterative Methods for Nonlinear (Scalar) Equations

$f(x) = 0$ solution

nonlinear function. $x \in [a, b]$.

$f(x) \in C[a, b]$

Section I. Bisection Method

a —— b. Assume $f(a)f(b) < 0$.

Let $c = \frac{a+b}{2}$. If $f(a)f(c) > 0$, replace a with c; otherwise, replace b with c.

Specify a tolerance $\varepsilon > 0$ for an iterative method.
e.g. $\varepsilon = 10^{-6}$. 10^{-8}. 10^{-10}

①. do {
step 1. $c = \frac{a+b}{2}$
step 2. if $f(a)f(c) > 0$, $a = c$; else $b = c$;
} while (fabs$(b-a) > \varepsilon$)
$x = c$.

②. while (fabs$(b-a) > \varepsilon$) {
step 1. $c = \frac{a+b}{2}$
step 2. if $f(a)f(c) > 0$, $a = c$; else $b = c$;

}

$c = \frac{a+b}{2}$; $x = c$,

Example : $f(x) = x - e^{-x}$ $[-1, 1]$.

$x^* \approx 0.567143$.

Section II. Fixed Point Method.

$$f(x) = 0.$$

x_0 : initial guess. $x_0 \to x_1 \to x_2 \to \cdots$

a sequence of approximate solutions.

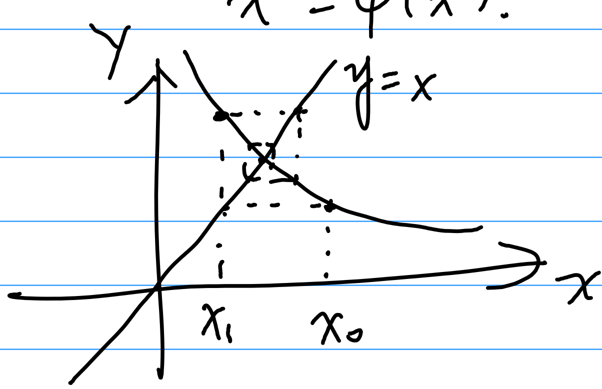
Let $k = 0, 1, 2 \cdots$

$$x_{k+1} \leftarrow \varphi(x_k)$$

If the sequence $\{x_k\}$ converges to x^*,

the limit x^* is a fixed point of the iterat or the function $\varphi(x)$.

$x^* = \varphi(x^*)$. $\Leftarrow \lim_{k \to +\infty} x_{k+1} = \lim_{k \to +\infty} \varphi(x_k)$.



If $\varphi(x) \in C[a,b]$, and $\varphi(x) \in [a,b]$,

then $\varphi(x)$ has a fixed point on $[a,b]$.

Let $f(x) = x - \varphi(x)$. $\quad a \le \varphi(x) \le b$

$$f(a) = a - \varphi(a) \le 0$$

$$f(b) = b - \varphi(b) \ge 0$$

1). $f(a) = 0 \Rightarrow a$ is a fixed point

2). $f(b) = 0 \Rightarrow b$ is a fixed point.

3) $f(a) < 0$. $f(b) > 0$

$f(x)$ has a zero x^* in the interval

i.e $f(x^*) = x^* - \varphi(x^*) = 0. \Rightarrow x^* = \varphi(x^*)$

If $|\varphi(x) - \varphi(y)| < L|x-y|$ with $L \in (0,1)$.

compression.

then the fixed point is unique

and the sequence $\{x_k\}$ generated by the iterate

$$x_{k+1} = \varphi(x_k) \qquad k = 0, 1, 2 \cdots$$

is convergent.

proof: If the fixed point is not unique. i.e.

$$\begin{cases} x^* = \varphi(x^*) \\ x^{**} = \varphi(x^{**}) \end{cases}$$

$$|x^* - x^{**}| = |\varphi(x^*) - \varphi(x^{**})| < L|x^* - x^{**}|$$

$$(1-L)|x^* - x^{**}| < 0 \quad \Rightarrow \text{contradiction}$$

$$|x_{k+1} - x_k| = |\varphi(x_k) - \varphi(x_{k-1})| \leq L|x_k - x_{k-1}|$$

$$\leq L^k |x_1 - x_0|. \qquad k > 0.$$

$$\Rightarrow |x_{k+p} - x_k| \leq \sum_{i=k}^{k+p-1} |x_{i+1} - x_i| \leq \sum_{i=k}^{k+p-1} L^i \cdot |x_1 - x_0|$$

$$\leq |x_1 - x_0| \cdot \sum_{i=k}^{k+p-1} L^i \leq \frac{L^k}{1-L} |x_1 - x_0|$$

$\Rightarrow \{x_k\}$ Cauchy seq. $\Rightarrow$ converged

If $\varphi(x) \in C^1[a,b]$. $\varphi(x) \in [a,b]$

and $|\varphi'(x)| \leq L$ $\quad L \in (0,1)$.

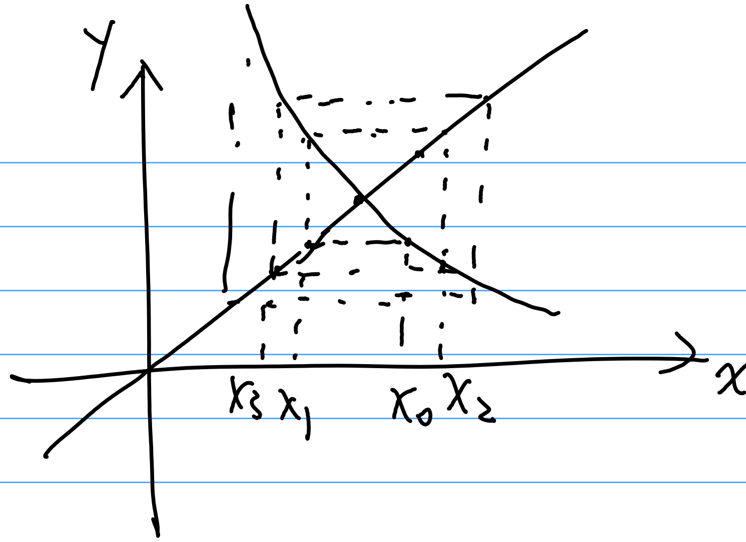
the funct $\varphi(x)$ has a unique fixed-point and the seq. $\{x_k\}$ generated by

$$x_{k+1} = \varphi(x_k)$$

converges to the fixed-point

$$\varphi(x) - \varphi(y) = \varphi'(\xi)(x-y)$$

$$\Rightarrow |\varphi(x) - \varphi(y)| = |\varphi'(\xi)| \cdot |x-y| \leq L|x-y|$$



Example 2. $f(x) = x - e^{-x} = 0$

$x - \varphi(x) = 0$. ① $\Rightarrow$ $f(x) = x - \varphi(x)$.

$\varphi(x) = x - f(x)$.

② $f(x) = \varphi(x) - x$. $\varphi(x) = x + f(x)$

③ $x - \varphi(x) = p(x) f(x)$ $\Rightarrow$ $\varphi(x) = x - p(x) f(x)$

preconditioner.

$-L < \varphi'(x) = 1 - p'(x) f(x) - p(x) f'(x) \leq L$

$1 - L \leq p'(x) f(x) + p(x) f'(x) \leq L + 1$.

if $p(x)$ constant, $p'(x) = 0$

$0 < 1 - L \leq p \cdot f'(x) \leq L + 1$

$1 - L \leq p f'(x) \leq L + 1$

$\varphi(x) = e^{-4x}$ $x = \varphi(x)$

Aitken technique (acceleration)

$$x_{n+1} = \varphi(x_n) \qquad \text{Let } x^* = \lim x_n .$$

error $\quad x^* - x_{n+1} = e_{n+1}$.

$x^* - x_n = e_n$.

$$e_{n+1} = x^* - x_{n+1} = \varphi(x^*) - \varphi(x_n) \approx \varphi'(\xi_n)(x^* - x_n)$$

With ξ_n be in the middle of x^* and x_n

provided that $\varphi(x)$ is continuously differentiable in a neighborhood of x^*

As ξ_n is (assumed to be) close to x^*,

we may treat $\varphi'(\xi_n)$ as a constant, c.

$$e_{n+1} \approx \varphi'(\xi_n)(x^* - x_n) = \varphi'(\xi_n) e_n \approx c e_n .$$

$$e_{n+1} = c e_n \qquad n = 0, 1, 2, \cdots$$

$$\begin{cases} e_1 \approx c e_0 \\ e_2 \approx c e_1 \end{cases} \Rightarrow \begin{cases} x^* - x_1 \approx c(x^* - x_0) \\ x^* - x_2 \approx c(x^* - x_1) \end{cases}$$

$$\frac{x^* - x_2}{x^* - x_1} \approx \frac{x^* - x_1}{x^* - x_0} \Rightarrow (x^* - x_1)^2 \approx (x^* - x_2)(x^* - x_0)$$

$$\Rightarrow x_1^2 - 2x^* x_1 \quad x_0 \cdot x_2 - (x_2 + x_0) x^*$$

$$\Rightarrow \quad x^* \approx \frac{x_1^2 - x_0 x_2}{2x_1 - (x_0 + x_2)}$$

It is reasonable to take $z = \dfrac{x_1^2 - x_0 x_2}{2x_1 - x_0 - x_2}$ as a more accurate approximation of x^* than x_0, x_1, x_2.

Accelerated iteration: for $k = 0, 1, 2 \ldots$

step 1. Let $y_0 = x_k$, $y_1 = \varphi(y_0)$, $y_2 = \varphi(y_1)$

$$x_{k+1} = \frac{y_1^2 - y_0 y_2}{2y_1 - y_0 - y_2}$$

step 2. Check if $|x_{k+1} - \varphi(x_{k+1})|$ is less than some prespecified tolerance ε. If it is, stop the iteration; otherwise, go back to step 1.

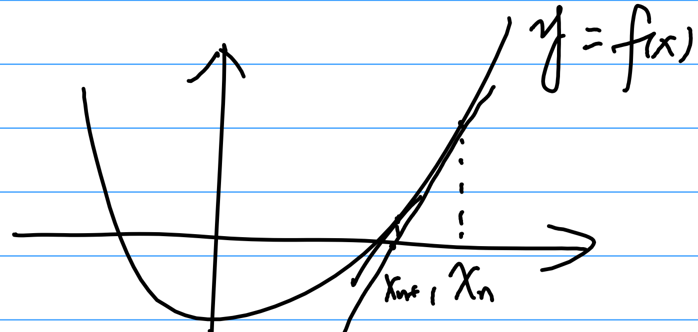
Remark: One may check $|x_{k+1} - x_k|$ to determine whether to stop the iteration.

Example 2. $f(x) = e^x - x - 1 = 0$.

$x = \varphi(x) = x + f(x)$ $\qquad \varphi'(x) = e^x$.

Section 3. Newton Iteration.

x_n.



linearization.

Approximate the curve around x_n with the tangent passing through $(x_n, f(x_n))$.

$$l(x) = f(x_n) + f'(x_n)(x - x_n).$$

Find the intersection of the tangent line with the x-axis.

i.e. $$l(x_{n+1}) = f(x_n) + f'(x_n)(x_{n+1} - x_n) = 0$$

$$\Rightarrow \quad x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \quad \text{for } n = 0, 1, 2 \ldots$$

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

The Newton method itself is a fixed point iteration. $x_{n+1} = \varphi(x_n)$.

$$\varphi'(x) = 1 - \frac{[f'(x)]^2 - f(x)f''(x)}{[f'(x)]^2} = \frac{f(x)f''(x)}{[f'(x)]^2}.$$

$f(x) \in C^2[a, b]$. twice continuously differentiable.

Observation: When (as long as) the initial guess is sufficiently close to a zero-point of $f(x)$, the Newton iterate converges, provided that $|f'(x)|$ and $|f''(x)|$ have reasonable size.

Convergence by checking error propagation

error $e_n = x^* - x_n$.

$$0 = f(x_{n+1}) = f(x_n) + f'(x_n)(x_{n+1} - x_n). \qquad (1)$$

$$0 = f(x^*) = f(x_n) + f'(x_n)(x^* - x_n) + \frac{1}{2} f''(\xi_n)(x^* - x_n)^2. \qquad (2)$$

(2) − (1) : $\quad 0 = f'(x_n)(x^* - x_{n+1}) + \frac{1}{2} f''(\xi_n)(x^* - x_n)^2$

$$f'(x_n)\, e_{n+1} = -\frac{1}{2} f''(\xi_n)\, e_n^2.$$

$$e_{n+1} = -\frac{1}{2}\frac{f''(\xi_n)}{f'(x_n)} e_n^2. \qquad (3)$$

The Newton iteration is a quadratic method.

(Convergence rate 2) → quadratic

Condition: The coefficient $\frac{f''(\xi_n)}{f'(x_n)}$ is approximately constant.

$$f(x_n) = f(x_n) - f(x^*) = f'(\eta_n)(x_n - x^*) = -f'(\eta_n)\, e_n$$

Example. $\quad f(x) = (1+x)(1-x)^2$.

Example. $\quad f(x) = x(x^2-2)+2$.

Example. $\quad f(x) = x^3 - x - 3$

Example. $\quad f(x) = \begin{cases} \sqrt{x} & x \geq 0 \\ -\sqrt{|x|} & x < 0. \end{cases}$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

$$f'(x) = \frac{1}{2}\frac{1}{\sqrt{x}} \qquad x > 0.$$

$$x_{n+1} = x_n - \frac{\sqrt{x_n}}{\frac{1}{2}\frac{1}{\sqrt{x_n}}} = x_n - 2x_n = -x_n$$

Example. $f(x) = xe^{-x}$.

By the examples, we see that the Newton method is not guaranted to converge

Convergence : 1). twice continuously differentiable

2). good initial guess

? How about the multiplicity of the root of $f(x)=0$ is greater than 1.

Assume x^* is a zero of $f(x)$ with multiplicity $p>1$.

i.e. $f(x) = (x-x^*)^p h(x) \qquad h(x^*) \neq 0$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \equiv \varphi(x_n)$$

$$\varphi(x) = x - \frac{f(x)}{f'(x)} = x - \frac{(x-x^*)^p h(x)}{p(x-x^*)^{p-1}h(x) + (x-x^*)^p h'(x)}$$

$$= x - \frac{(x-x^*)h(x)}{ph(x) + (x-x^*)h'(x)}$$

$$\varphi'(x^*) = 1 - \frac{h^2(x^*)\cdot p}{p^2 h^2(x^*)} = 1-\frac{1}{p} \in (0,1).$$

The iteration just converges linearly.
(not quadratically)

The Newton method with damping.

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \quad n=0,1,2\cdots$$

Let $\delta_n = -\frac{f(x_n)}{f'(x_n)}$. We call δ_n as the Newton step.

$$x_{n+1} = x_n + \delta_n$$

$$g(x) = \frac{1}{2} f^2(x).$$

$$g(x) = g(x^* + \lambda(\underline{x-x^*}))$$

$$\varphi(\lambda) = g(x_n+\lambda\delta_n) \quad \checkmark \qquad (\lambda \geq 0)$$

$$\varphi'(\lambda)\Big|_{\lambda=0} = f(x_n+\lambda\delta_n)f'(x_n+\lambda\delta_n)\delta_n\Big|_{\lambda=0}$$

$$= f(x_n)f'(x_n)\delta_n = -f(x_n)f'(x_n)\cdot\frac{f(x_n)}{f'(x_n)} = -f^2(x_n)$$

$$< 0$$

$$\varphi(\lambda) \approx \varphi(0) + \varphi'(0)\lambda \qquad \varphi'(0)<0$$

When λ is small (sufficiently small)

$$\varphi(\lambda) < \varphi(0)$$

In the Newton iteration with damping, we introduce a parameter λ_n.

$$x_{n+1} = x_n + \lambda_n \delta_n.$$

so that $\quad g(x_{n+1}) < g(x_n) \qquad (*)$

step 0. Let $\lambda_n = 1$

step 1 Let $z_{n+1} = x_n + \lambda_n \delta_n$

step 2. check if $|f(z_{n+1})| < |f(x_n)|$. $\qquad$ (1).

If $|f(z_{n+1})| \geq |f(x_n)|$, set $\lambda_n \leftarrow \lambda_n/2$ and go back to step 1.; otherwise.

let $x_{n+1} = z_{n+1}$.

Remark: ① For different functions, one may add extra checking. For example, if $f(x) = x \ln(x)$. one need to check if

$z_{n+1} > 0$

② In order to avoid working with too small steps, one should stop the iteration for damping after a few times (say, 4-6).

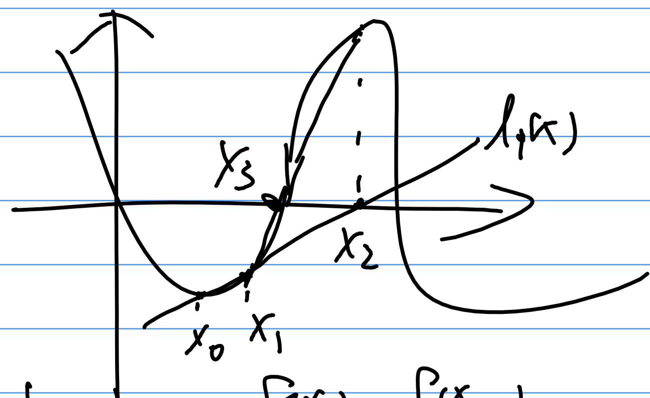
The method is also called a modified Newton method.

Optimize $g(x)$: $g'(x) = 0$

$$x_{n+1} = x_n - \frac{g'(x_n)}{g''(x_n)}$$

$g''(x_n) > 0$? < 0 ?

Section 4. The Secant Method.



$$f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

Locally, approximate the function $f(x)$ with a secant line

$$l(x) = f(x_n) + \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}} (x - x_n)$$

Choose x_{n+1} so that $l(x_{n+1}) = 0$

$$x_{n+1} = x_n - \frac{f(x_n)}{\frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}} \qquad n = 1, 2, \cdots$$

provided that two initial guess x_0, x_1 are given.

$$f(x) = (x-1)\exp\left(-\frac{1}{(1-x)^2}\right)$$