數值分析 MA-3021

Chapter 2. Solutions of Nonlinear Equations

§2.1 Bisection Method

§2.2 Fixed-Point Iteration and Error Analysis

§2.3 Newton's Method (for Equation of One Variable)

§2.4 Secant Method

§2.5 Newton's Method for System of Equations

Introduction

1. Let $f\colon \varnothing \neq A \subseteq \mathbb{R} \to \mathbb{R}$ be a nonlinear real-valued function in variable x. We are interested in finding the roots (solutions) of the equation $f(x) = 0$; i.e., zeros of the function $f(x)$.
2. **A system of nonlinear equations:**
   Let $F : \varnothing \neq A \subseteq \mathbb{R}^n \to \mathbb{R}^n$ be a nonlinear vector-valued function in a vector variable $X = (x_1, x_2, \cdots, x_n)^\top$. We are interested in finding the roots (solutions) of the equation $F(X) = \mathbf{0}$; i.e., zeros of the function $F(X)$.

Introduction

Example

- Let us look at three functions (polynomials):
  - $f(x) = x^4 - 12x^3 + 47x^2 - 60x$
  - $f(x) = x^4 - 12x^3 + 47x^2 - 60x + 24$
  - $f(x) = x^4 - 12x^3 + 47x^2 - 60x + 24.1$
- Find the zeros of these polynomials is not an easy task.
  - The first function has real zeros 0, 3, 4, and 5.
  - The real zeros of the second function are 1 and $0.888\ldots$.
  - The third function has no real zeros at all.
- Matlab: `p = [1 -12 47 -60 0]; r = roots(p)`

Introduction

Consider the nonlinear equation $f(x) = 0$ or $F(X) = \mathbf{0}$.

- The basic questions:
  - Does the solution exist?
  - Is the solution unique?
  - How to find it?
- In this lecture, we will mainly focus on the third question and we always assume that the problem under considered has a solution x^*.
- We will study iterative methods for finding the solution: first find an initial guess x_0, then a better guess $x_1, \cdots$, in the end we hope that $\lim_{n\to\infty} x_n = x^*$.

Introduction

- Iterative methods: **Constructive** ways of finding roots of equations
  - Bisection method;
  - Fixed-point method;
  - Newton's method;
  - Secant method.

§2.1 Bisection Method

Theorem (Bolzano)

Let $f : [a, b] \to \mathbb{R}$ be continuous. If $f(a)f(b) < 0$, then there exists $c \in (a, b)$ such that $f(c) = 0$.

The basic idea: Assume that $f(a)f(b) < 0$.

- Set $a_1 = a$ and $b_1 = b$, compute $p_1 = \frac{1}{2}(a_1 + b_1)$.
- If $f(p_1)f(a_1) = 0$ then $f(p_1) = 0 \Rightarrow p = p_1$;

  if $f(p_1)f(a_1) > 0$ then $p \in (p_1, b_1)$, set $a_2 = p_1$ and $b_2 = b_1$;

  if $f(p_1)f(a_1) < 0$ then $p \in (a_1, p_1)$, set $a_2 = a_1$ and $b_2 = p_1$.
- $p_2 = \frac{1}{2}(a_2 + b_2)$.
- Repeat the process until the interval is very small then any point in the interval can be used as approximations of the zero. In fact, $p_1 \rightharpoonup p_2 \rightharpoonup p_3 \rightharpoonup \cdots \rightharpoonup p$.

The bisection algorithm

Input a, b, tolerance TOL, max. no. of iteration N_0.

Output approximate sol. of p or message of failure.

Step 1: $i = 1$, $FA = f(a)$.

Step 2: while $i \leqslant N_0$ do step 3-6.

Step 3: set $p = a + \frac{1}{2}(b - a)$; $FP = f(p)$.

Step 4: if $FP = 0$ or $\frac{1}{2}(b - a) < TOL$ then output(p); stop.

Step 5: $i = i + 1$.

Step 6: if $FA \times FP > 0$ then set $a = p$ and $FA = FP$;

else set $b = p$.

Step 7: output (method failed after N_0 iterations); stop.

The bisection algorithm

Input a, b, tolerance TOL, max. no. of iteration N_0.

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Step 1: $i = 1$, $FA = f(a)$.

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Step 7: output (method failed after N_0 iterations); stop.

§2.1 Bisection Method

Stopping criteria

- The stopping criteria are practical tests needed to determine when to stop the iteration (loop) or even the whole program. In our algorithm in the previous page, two stopping criteria are

$$FP = 0 \qquad \text{or} \qquad \frac{1}{2}(b-a) < TOL\,.$$

- Let $\varepsilon > 0$ be a given tolerance.
  - The stopping criterium $FP = 0$ can be replaced by $|FP| < \varepsilon$.
  - The stopping criterium $\frac{1}{2}(b-a) < TOL$ can be replaced by

$$|p_i - p_{i-1}| < \varepsilon \qquad \text{or} \qquad \frac{|p_i - p_{i-1}|}{p_i} < \varepsilon\,.$$

Example

Find a root of $f(x) = x^3 + 4x^2 - 10$.

Note that $f(1) = -5$, $f(2) = 14$. Therefore, there exists a root $p \in [1, 2]$. Actual root is $p = 1.365230013\ldots$

Using the bisection method, we get the table:

n	a_n	b_n	p_n	$f(p_n)$
1	1.000000000000	2.000000000000	1.500000000000	2.375000000000
2	1.000000000000	1.500000000000	1.250000000000	-1.796875000000
3	1.250000000000	1.500000000000	1.375000000000	0.162109375000
⋮	⋮	⋮	⋮	⋮
13	1.364990234375	1.365234375000	1.365112304687	-0.001943659010
14	1.365112304687	1.365234375000	1.365173339843	-0.000935847281
⋮	⋮	⋮	⋮	⋮
18	1.365226745605	1.365234375000	1.365230560302	0.000009030992

See the details of the M-file: `bisection.m`

§2.1 Bisection Method

Properties of bisection methods

- **Drawbacks:**
  - often slow;
  - a good intermediate approximation may be discarded;
  - doesn't work for higher dimensional problems: $F(X) = \mathbf{0}$.
- **Advantage:** it always converges to a solution if a suitable initial interval can be chosen.

§2.1 Bisection Method

Theorem

If $f \in C([a,b])$ and p is the unique zero of f in $[a,b]$, then the bisection method generates $\{p_n\}_{n=1}^{\infty}$ with $|p_n - p| \leqslant \frac{1}{2^n}(b-a)$ for all $n \geqslant 1$.

Proof.

For $n \geqslant 1$, we have $b_n - a_n = \frac{1}{2^{n-1}}(b-a)$ and $p \in [a_n, b_n]$.

$\because\ p_n = \frac{1}{2}(a_n + b_n),\ \forall\ n \geqslant 1.$

$\therefore\ |p_n - p| \leqslant \frac{1}{2}(b_n - a_n) = \frac{1}{2} \cdot \frac{1}{2^{n-1}}(b-a) = \frac{1}{2^n}(b-a).$ □

Note: Since $|p_n - p| \leqslant \frac{1}{2^n}(b-a)$, we have $p_n = p + \mathcal{O}\left(\frac{1}{2^n}\right)$.

§2.2 Fixed-Point Iteration and Error Analysis

Definition

Let $\varnothing \neq X \subseteq Y$ be two sets, and $g: X \to Y$ be a function. A point $p \in X$ is called a fixed-point of g if $g(p) = p$.

Root-finding problem & fixed-point problem are equivalent in the following sense:

- If p is a root of $f(x) = 0$, p is a fixed point of $g(x) := x - f(x)$, $h(x) := x - \dfrac{f(x)}{f'(x)}$, and etc.
- If p is a fixed point of $g(x)$; i.e., $g(p) = p$, then p is a root of $f(x) := x - g(x)$, $h(x) := 3x - 3g(x)$, and etc.

(root-finding problem) $\Leftrightarrow$ (fixed-point problem).

§2.2 Fixed-Point Iteration and Error Analysis

Example

Let $g : [-2, 3] \to \mathbb{R}$ be defined by $g(x) = x^2 - 2$.

$\because g(-1) = (-1)^2 - 2 = -1$ and $g(2) = 2^2 - 2 = 2$.

$\therefore -1$ and 2 are fixed points of g.

Moreover,finding the fixed-point of g is equivalent to finding the zeros of the function $f(x) = x^2 - x - 2$.

§2.2 Fixed-Point Iteration and Error Analysis

Theorem

Let $-\infty < a < b < \infty$ and $g : [a, b] \to [a, b]$ be continuous. Then g has a fixed-point.

Proof.

If $g(a) = a$ or $g(b) = b$ then g has a fixed point in $[a, b]$. Suppose not, then $a < g(a) \leqslant b$ and $a \leqslant g(b) < b$. Define $h(x) := g(x) - x$. Then h is continuous on $[a, b]$ and $h(a) > 0$, $h(b) < 0$. By the Intermediate Value Theorem, there exists $p \in (a, b)$ such that $h(p) = 0$; i.e., $g(p) = p$. □

Example

Let $g : [-2, 2] \to \mathbb{R}$ be defined by $g(x) = x^2 - 2$. Then $g : [-2, 2] \to [-2, 2]$ and -1 and 2 are fixed points of g.

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§2.2 Fixed-Point Iteration and Error Analysis

Theorem (Banach fixed-point theorem)

Let $-\infty < a < b < \infty$ and $g : [a, b] \to [a, b]$. If there exists a constant $k \in [0, 1)$ such that

$$|g(x) - g(y)| \leqslant k|x - y| \qquad \forall\, x, y \in [a, b]\,,$$

then there exists a unique fixed-point of g (i.e., there is one and only one fixed-point of g). Moreover, for any given $p_1 \in [a, b]$, the sequence $\{p_n\}_{n=1}^{\infty}$ obtained by $p_{n+1} = g(p_n)$ for all $n \in \mathbb{N}$ converges to the fixed-point p and

$$|p_n - p| \leqslant k^{n-1}|p_1 - p| \quad \text{and} \quad |p_n - p| \leqslant \frac{k^{n-1}}{1-k}|p_2 - p_1|\,. \qquad (\star)$$

Note: Even though we might not know where p locates, $(\star)$ is still a good estimate of the speed of convergence of $\{p_n\}_{n=1}^{\infty}$ to p.

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§2.2 Fixed-Point Iteration and Error Analysis

Proof.

Note that the condition $|f(x) - f(y)| \leqslant k|x - y|$ for all x, y in $[a, b]$ implies that f is continuous on $[a, b]$; thus the previous theorem implies that f has at least one fixed-point.

Suppose that p and q are fixed-points of g. Then

$$|p - q| = |g(p) - g(q)| \leqslant k|p - q|.$$

Since $k \in [0, 1)$, we must have $|p - q| = 0$ or $p = q$. Therefore, there is only one fixed-point of g.

Let $p_1 \in [a, b]$, and $p_{n+1} = g(p_n)$ for all $n \in \mathbb{N}$. Then

$$|p_{n+1} - p| = |g(p_n) - g(p)| \leqslant k|p_n - p| \qquad \forall\, n \geqslant 1.$$

Therefore,

$$|p_n - p| \leqslant k|p_{n-1} - p| \leqslant k^2|p_{n-2} - p| \leqslant \cdots \leqslant k^{n-1}|p_1 - p|;$$

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§2.2 Fixed-Point Iteration and Error Analysis

Goal: $|p_n - p| \leqslant \dfrac{k^{n-1}}{1-k}|p_2 - p_1|$ for all $n \geqslant 2$.

Proof (Cont.)

Finally, we note that

$$|p_{n+1} - p_n| = \big|g(p_n) - g(p_{n-1})\big| \leqslant k|p_n - p_{n-1}| \quad \forall\, n \geqslant 2;$$

thus if $n + j \geqslant 2$,

$$\begin{aligned}|p_{n+j} - p_{n+j-1}| &\leqslant k|p_{n+j-1} - p_{n+j-2}| \leqslant k^2|p_{n+j-2} - p_{n+j-3}| \\ &\leqslant \cdots \leqslant k^{n+j-2}|p_2 - p_1|\,.\end{aligned}$$

Therefore, for $j \geqslant 1$ and $n \geqslant 2$,

$$\begin{aligned}|p_{n+j} - p_n| &\leqslant |p_{n+j} - p_{n+j-1}| + \cdots + |p_{n+2} - p_{n+1}| + |p_{n+1} - p_n| \\ &\leqslant (k^j + k^{j-1} + \cdots + k)k^{n-2}|p_2 - p_1| \\ &\leqslant \frac{1-k^j}{1-k}k^{n-1}|p_2 - p_1|\,.\end{aligned}$$

The final conclusion follows from passing to the limit as $j \to \infty$. □

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Theorem (Banach fixed-point theorem)

Let $-\infty < a < b < \infty$ and $g : [a, b] \to [a, b]$. If there exists a constant $k \in [0, 1)$ such that

$$\big|g(x) - g(y)\big| \leqslant k|x - y| \qquad \forall\, x, y \in [a, b]\,,$$

then there exists a unique fixed-point of g (i.e., there is one and only one fixed-point of g). Moreover, for any given $p_1 \in [a, b]$, the sequence $\{p_n\}_{n=1}^{\infty}$ obtained by $p_{n+1} = g(p_n)$ for all $n \in \mathbb{N}$ converges to the fixed-point p and

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Definition

Let $\varnothing \neq A \subseteq \mathbb{R}^n$. A function $g : A \to \mathbb{R}^n$ is called a contraction or a contraction mapping if there exists a constant $k \in [0, 1)$ such that

$$\big\|g(x) - g(y)\big\| \leqslant k\|x - y\| \qquad \forall\, x, y \in A\,.$$

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§2.2 Fixed-Point Iteration and Error Analysis

Theorem (Contraction mapping principle)

Let $-\infty < a < b < \infty$ and $g : [a, b] \to [a, b]$. If there exists a constant $k \in [0, 1)$ such that

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$$|p_n - p| \leqslant k^{n-1}|p_1 - p| \quad \text{and} \quad |p_n - p| \leqslant \frac{k^{n-1}}{1-k}|p_2 - p_1|\,. \qquad (\star)$$

Definition

Let $\varnothing \neq A \subseteq \mathbb{R}^n$. A function $g : A \to \mathbb{R}^n$ is called a contraction or a contraction mapping if there exists a constant $k \in [0, 1)$ such that

$$\left\|g(x) - g(y)\right\| \leqslant k\|x - y\| \qquad \forall\, x, y \in A\,.$$

§2.2 Fixed-Point Iteration and Error Analysis

Theorem

Let $I \subseteq \mathbb{R}$ be an interval, and $f : I \to \mathbb{R}$. If there exists a constant $k \in [0, 1)$ such that $|f'(x)| \leqslant k$ for all $x \in I$, then f is a contraction.

Proof.

Let $x, y \in I$. By MVT, there exists z between x and y such that

$$f(x) - f(y) = f'(z)(x - y);$$

thus by the condition that $|f'(x)| \leqslant k$ for all $x \in I$,

$$|f(x) - f(y)| = |f'(z)||x - y| \leqslant k|x - y|.$$

Since $k < 1$, f is a contraction. □

Example

The function $f : (0, \infty) \to \mathbb{R}$ defined by $f(x) = \arctan x$ is not a contraction even though $|f'(x)| < 1$ for all $x \in \mathbb{R}$.

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§2.2 Fixed-Point Iteration and Error Analysis

Fixed point iterations

$$p_n = g(p_{n-1}), \quad n = 1, 2, \cdots$$

Assume that g is continuous and $\lim_{n\to\infty} p_n = p$. Then

$$g(p) = g\left(\lim_{n\to\infty} p_n\right) = g\left(\lim_{n\to\infty} p_{n-1}\right) = \lim_{n\to\infty} g(p_{n-1})$$
$$= \lim_{n\to\infty} p_n = p.$$

Therefore, p is a fixed point of the function g.

Note: When g is continuous, the iteration scheme $p_{n+1} = g(p_n)$ in general will **NOT** produce a convergent sequence $\{p_n\}_{n=1}^{\infty}$.

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§2.2 Fixed-Point Iteration and Error Analysis

Example

The function $f(x) = x^3 + 4x^2 - 10$ has a unique zero in $[1, 2]$:

1. Since $f(1) = -5 < 0$ and $f(2) = 14 > 0$, Bolzano's Theorem implies that f has a zero in $[1, 2]$.
2. Since $f'(x) = 3x^2 + 8x > 0$ for all $x \in (1, 2)$, f is strictly increasing on $[1, 2]$; f has a unique zero in $[1, 2]$.

Next, we focus on finding the unique zero of f using the fixed-point iteration. This amounts to provide a **good** continuous function g so that $x = g(x)$ is equivalent to $f(x) = 0$.

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§2.2 Fixed-Point Iteration and Error Analysis

Example (Cont.)

Some computations show that the fixed-point of the following functions are the unique zero of f.

(a) $x = g_1(x) := x - x^3 - 4x^2 + 10.$

(b) $x = g_2(x) := \left(\frac{10}{x} - 4x\right)^{1/2}.$

(c) $x = g_3(x) := \frac{1}{2}\left(10 - x^3\right)^{1/2}.$

(d) $x = g_4(x) := \left(\frac{10}{4+x}\right)^{1/2}.$

(e) $x = g_5(x) := x - \frac{x^3 + 4x^2 - 10}{3x^2 + 8x}.$

§2.2 Fixed-Point Iteration and Error Analysis

Example (Cont.)

Using the fixed-point iterations with functions $g_1, g_2, \cdots, g_5$ and $p_0 = 1.5$, we have the following numerical results:

n	(a)	(b)	(c)	(d)	(e)
0	1.5	1.5	1.5	1.5	1.5
⋮	⋮	⋮	⋮	⋮	⋮
3	-469.7	$(-8.65)^{1/2}$			
4	1.03×10^8				1.365230013
			⋮	⋮	
15			1.365223680	1.365230013	
			⋮		
30			1.365230013		

The actual root is $p = 1.365230013...$

Computer project: write the Matlab files for (c), (d), and (e).

§2.2 Fixed-Point Iteration and Error Analysis

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§2.3 Newton's Method

- **Motivation:** we know how to solve $f(x) = 0$ if f is linear. For nonlinear f, we can always approximate it with a linear function.
- Suppose that $f \in C^2([a, b])$ and $f(p) = 0$. Let $p_0 \in [a, b]$ be an approximation to p, $f'(p_0) \neq 0$ and $|p - p_0|$ is "small". Using Taylor Theorem, we have

$$0 = f(p) = f(p_0) + (p - p_0)f'(p_0) + \frac{(p - p_0)^2}{2} f''(\xi(p)) .$$

If $|p - p_0|$ is small, then we can drop the $(p - p_0)^2$ term,

$$0 \approx f(p_0) + (p - p_0)f'(p_0) .$$

Solving for p gives

$$p \approx p_1 := p_0 - \frac{f(p_0)}{f'(p_0)}, \quad \text{provided} \quad f'(p_0) \neq 0 .$$

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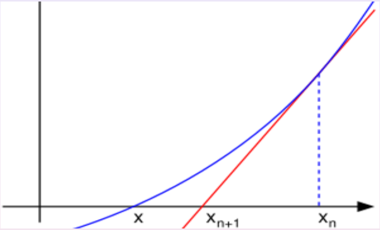
- **Newton's method** can be defined as follows: for $n = 0, 1, 2, \cdots$

$$p_{n+1} = p_n - \frac{f(p_n)}{f'(p_n)}, \quad \text{provided} \quad f'(p_n) \neq 0 .$$

§2.3 Newton's Method

Geometrical interpretation



- An illustration of one iteration of Newton's method. The function f is shown in blue and the tangent line is in red. We see that p_{n+1} is a better approximation than p_n for the root p of the function f.
- What is the geometrical meaning of $f'(p_n) = 0$?

§2.3 Newton's Method

Example

Find the zero the function $f(x) = \cos x - x$ in $[0, \pi/2]$.

- $\because$ $f(\pi/2) = -\pi/2 < 0$ and $f(0) = 1 > 0$.

  $\therefore$ there exists $p \in (0, \pi/2)$ such that $f(p) = 0$.

  Newton's method: choose $p_0 \in [0, \pi/2]$ and

$$p_n := p_{n-1} - \frac{\cos(p_{n-1}) - p_{n-1}}{-\sin(p_{n-1}) - 1}, \quad n \geqslant 1.$$

- **Numerical results:** $p_0 = \pi/4$.

n	p_n	$f(p_n)$
0	0.78539816339745	-0.07829138221090
1	0.73953613351524	-0.00075487468250
2	0.73908517810601	-0.00000007512987
3	0.73908513321516	-0.00000000000000

§2.3 Newton's Method

Theorem

Assume that $f \in C^2([a,b])$, $p \in (a,b)$ *such that* $f(p) = 0$ *and* $f'(p) \neq 0$. *Then there exists* $\delta > 0$ *such that if* $p_0 \in [p-\delta, p+\delta]$ *then Newton's method generates* $\{p_n\}_{n=1}^{\infty}$ *converging to* p.

Idea of proof: Define $g(x) = x - \dfrac{f(x)}{f'(x)}$. Then p is a fixed-point of g. To apply the Banach fixed-point theorem for the construction of the fixed-point of g, we want to find $\delta > 0$ such that

1. $g : [p-\delta, p+\delta] \to [p-\delta, p+\delta]$ or equivalently,
$$\left|g(x) - p\right| \leqslant \delta \quad \forall\, x \in [p-\delta, p+\delta].$$
2. there exists $k \in (0,1)$ such that $|g'(x)| \leqslant k$ for all $x \in [p-\delta, p+\delta]$.

§2.3 Newton's Method

Proof.

Since f' is continuous on $[a, b]$, there exists $\delta_1 > 0$ such that

$$\left|f'(p) - f'(x)\right| < \frac{\left|f'(p)\right|}{2} \quad \forall\, x \in [p-\delta_1, p+\delta_1] \subseteq [a, b]\,.$$

Let $k \in (0, 1)$ be a constant and $g : [p-\delta_1, p+\delta_1] \to \mathbb{R}$ be defined by $g(x) = x - \dfrac{f(x)}{f'(x)}$. Then

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

Therefore, g' is continuous on $[p-\delta_1, p+\delta_1]$. Moreover, $g'(p) = 0$; thus there exists $0 < \delta < \delta_1$ such that

$$\left|g'(x)\right| \leqslant k \quad \forall\, x \in [p-\delta, p+\delta]\,.$$

The mean value theorem further implies that

$$\left|g(x) - p\right| = \left|g(x) - g(p)\right| \leqslant k|x-p| < \delta \quad \forall\, x \in [p-\delta, p+\delta]\,. \quad \square$$

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A sequence $\{p_n\}_{n=1}^{\infty}$ is said to converge to p of order α, where $\alpha > 0$, if $\lim_{n\to\infty} p_n = p$ and there exists $M > 0$ such that

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Assume that $f \in C^2([a,b])$, $p \in (a,b)$ such that $f(p) = 0$ and $f'(p) \neq 0$. If $\{p_n\}_{n=1}^{\infty}$ given by

$$p_{n+1} = p_n - \frac{f(p_n)}{f'(p_n)} \qquad \forall\, n \geqslant 1$$

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In short,

Newton's method is quadratically convergent when it converges.

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$$(p - p_n) + \frac{f(p_n)}{f'(p_n)} = -\frac{f''(\xi_n)}{2f'(p_n)}(p - p_n)^2$$

which implies that

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Since $f \in C^2([a, b])$ and $f(p) = 0$, by Taylor's Theorem for each $n \in \mathbb{N}$ there exists ξ_n between p and p_n such that

$$f(p_n) + f'(p_n)(p - p_n) = -\frac{f''(\xi_n)}{2!}(p - p_n)^2 .$$

Therefore,

$$(p - p_n) + \frac{f(p_n)}{f'(p_n)} = -\frac{f''(\xi_n)}{2f'(p_n)}(p - p_n)^2$$

which implies that

$$|p - p_{n+1}| \leqslant \frac{\max_{x\in[a,b]} |f''(x)|}{2|f'(p_n)|}|p - p_n|^2 \quad \text{for all} \quad n .$$

□

§2.3 Newton's Method

Theorem

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which implies that

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§2.3 Newton's Method

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$$p - p_{n+1} = -\frac{f''(\xi_n)}{2f'(p_n)}(p - p_n)^2$$

which implies that

$$|p - p_{n+1}| \leqslant \frac{\max\limits_{x\in[a,b]} |f''(x)|}{|f'(p)|} |p - p_n|^2 \quad \text{for all large } n .$$

□

§2.3 Newton's Method

Remark:

- **Advantages:**
  1. The convergence is quadratic.
  2. Newton's method works for higher dimensional problems.
- **Disadvantages:**
  1. Newton's method converges only locally; i.e., the initial guess p_0 has to be close enough to the solution p.
  2. It needs the first derivative of $f(x)$.

§2.4 Secant Method

- **Secant method:** given two initial approximations p_0 and p_1 with $p_0 \neq p_1$ and $f(p_0) \neq f(p_1)$. Then for $n \geqslant 2$,
  - compute $m = \dfrac{f(p_{n-1}) - f(p_{n-2})}{p_{n-1} - p_{n-2}}$, if $p_{n-1} \neq p_{n-2}$.
  - compute $p_n = p_{n-1} - \dfrac{f(p_{n-1})}{m}$, if $f(p_{n-1}) \neq f(p_{n-2})$.

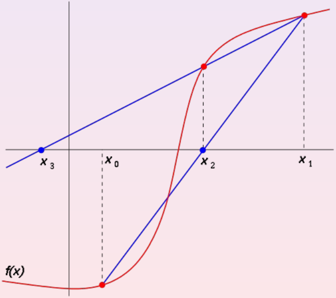

Figure 1: This picture is quoted from http://en.wikipedia.org/wiki/

§2.4 Secant Method

- **Remarks:**
  - we need only one function evaluation per iteration.
  - p_n depends on two previous iterations. For example, to compute p_2, we need both p_1 and p_0.
  - how do we obtain p_1? We need to use FD-Newton: pick a small parameter h, compute $a_0 = (f(p_0 + h) - f(p_0))/h$, then $p_1 = p_0 - f(p_0)/a_0$.
- The convergence of secant method is superlinear (i.e., better than linear). More precisely, we have

$$\lim_{n\to\infty} \frac{|p_{n+1} - p|}{|p_n - p|^{(1+\sqrt{5})/2}} = C, \quad (1+\sqrt{5})/2 \approx 1.62 < 2.$$

§2.4 Secant Method

Example

Find the zero the function $f(x) = \cos x - x$ in $[0, \pi/2]$.

- Let $p_0 = 0.5$ and $p_1 = \pi/4$.

  The secant method:

$$p_n := p_{n-1} - \frac{(p_{n-1} - p_{n-2})(\cos(p_{n-1}) - p_{n-1})}{(\cos(p_{n-1}) - p_{n-1}) - (\cos(p_{n-2}) - p_{n-2})}, \quad n \geqslant 2.$$

- **Numerical results:**

n	p_n	$f(p_n)$
0	0.50000000000000	0.37758256189037
1	0.78539816339745	-0.07829138221090
2	0.73638413883658	0.00451771852217
3	0.73905813921389	0.00004517721596
4	0.73908514933728	-0.00000002698217
5	0.73908513321506	0.00000000000016

§2.5 Newton's Method for System of Equations

We first focus on solving for zeros of system of two nonlinear equations. We wish to solve

$$\begin{cases} f_1(x_1, x_2) = 0, \\ f_2(x_1, x_2) = 0, \end{cases}$$

where f_1 and f_2 are nonlinear functions of x_1 and x_2.

Applying Taylor's expansion in two variables around (x_1, x_2) to the system of equations, we obtain

$$\begin{cases} 0 = f_1(x_1+h_1, x_2+h_2) \approx f_1(x_1, x_2) + h_1 \dfrac{\partial f_1(x_1, x_2)}{\partial x_1} + h_2 \dfrac{\partial f_1(x_1, x_2)}{\partial x_2}, \\ 0 = f_2(x_1+h_1, x_2+h_2) \approx f_2(x_1, x_2) + h_1 \dfrac{\partial f_2(x_1, x_2)}{\partial x_1} + h_2 \dfrac{\partial f_2(x_1, x_2)}{\partial x_2}. \end{cases}$$

Putting it into the matrix form, we have

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} \approx \begin{bmatrix} f_1(x_1, x_2) \\ f_2(x_1, x_2) \end{bmatrix} + \begin{bmatrix} \frac{\partial f_1(x_1,x_2)}{\partial x_1} & \frac{\partial f_1(x_1,x_2)}{\partial x_2} \\ \frac{\partial f_2(x_1,x_2)}{\partial x_1} & \frac{\partial f_2(x_1,x_2)}{\partial x_2} \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}.$$

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Applying Taylor's expansion in two variables around (x_1, x_2) to the system of equations, we obtain

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Putting it into the matrix form, we have

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} \approx \begin{bmatrix} f_1(x_1, x_2) \\ f_2(x_1, x_2) \end{bmatrix} + \begin{bmatrix} \frac{\partial f_1(x_1,x_2)}{\partial x_1} & \frac{\partial f_1(x_1,x_2)}{\partial x_2} \\ \frac{\partial f_2(x_1,x_2)}{\partial x_1} & \frac{\partial f_2(x_1,x_2)}{\partial x_2} \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}.$$

§2.5 Newton's Method for System of Equations

Newton's method for the system of two nonlinear equations is defined as follows: for $k = 0, 1, \cdots,$

$$\begin{bmatrix} x_1^{(k+1)} \\ x_2^{(k+1)} \end{bmatrix} = \begin{bmatrix} x_1^{(k)} \\ x_2^{(k)} \end{bmatrix} + \begin{bmatrix} h_1^{(k)} \\ h_2^{(k)} \end{bmatrix}$$

with

$$\begin{bmatrix} \frac{\partial f_1}{\partial x_1}(x_1^{(k)}, x_2^{(k)}) & \frac{\partial f_1}{\partial x_2}(x_1^{(k)}, x_2^{(k)}) \\ \frac{\partial f_2}{\partial x_1}(x_1^{(k)}, x_2^{(k)}) & \frac{\partial f_2}{\partial x_2}(x_1^{(k)}, x_2^{(k)}) \end{bmatrix} \begin{bmatrix} h_1^{(k)} \\ h_2^{(k)} \end{bmatrix} = - \begin{bmatrix} f_1(x_1^{(k)}, x_2^{(k)}) \\ f_2(x_1^{(k)}, x_2^{(k)}) \end{bmatrix}.$$

§2.5 Newton's Method for System of Equations

Example

Use Newton's method with initial guess

$$\mathbf{x}^{(0)} = (x_1^{(0)}, x_2^{(0)})^\top = (0, 1)^\top$$

to solve the following nonlinear system (perform two iterations):

$$\begin{cases} 4x_1^2 - x_2^2 = 0, \\ 4x_1 x_2^2 - x_1 = 1. \end{cases}$$

Let $f_1(x_1, x_2) = 4x_1^2 - x_2^2$ and $f_2(x_1, x_2) = 4x_1 x_2^2 - x_1 - 1$. Then

$$\begin{bmatrix} \frac{\partial f_1}{\partial x_1}(x_1, x_2) & \frac{\partial f_1}{\partial x_2}(x_1, x_2) \\ \frac{\partial f_2}{\partial x_1}(x_1, x_2) & \frac{\partial f_2}{\partial x_2}(x_1, x_2) \end{bmatrix} = \begin{bmatrix} 8x_1 & -2x_2 \\ 4x_2^2 - 1 & 8x_1 x_2 \end{bmatrix};$$

§2.5 Newton's Method for System of Equations

$f_1(x_1, x_2) = 4x_1^2 - x_2^2$, $f_2(x_1, x_2) = 4x_1 x_2^2 - x_1 - 1$, and

$$\begin{bmatrix} \frac{\partial f_1}{\partial x_1}(x_1, x_2) & \frac{\partial f_1}{\partial x_2}(x_1, x_2) \\ \frac{\partial f_2}{\partial x_1}(x_1, x_2) & \frac{\partial f_2}{\partial x_2}(x_1, x_2) \end{bmatrix} = \begin{bmatrix} 8x_1 & -2x_2 \\ 4x_2^2 - 1 & 8x_1 x_2 \end{bmatrix};$$

thus the first iteration gives

$$\begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} + \begin{bmatrix} h_1^{(0)} \\ h_2^{(0)} \end{bmatrix}$$

$$= \begin{bmatrix} 0 \\ 1 \end{bmatrix} - \begin{bmatrix} 8 \cdot 0 & -2 \cdot 1 \\ 4 \cdot 1^2 - 1 & 8 \cdot 0 \cdot 1 \end{bmatrix}^{-1} \begin{bmatrix} f_1(0, 1) \\ f_2(0, 1) \end{bmatrix}$$

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thus the first iteration gives

$$\begin{aligned} \begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \end{bmatrix} &= \begin{bmatrix} 0 \\ 1 \end{bmatrix} + \begin{bmatrix} h_1^{(0)} \\ h_2^{(0)} \end{bmatrix} \\ &= \begin{bmatrix} 0 \\ 1 \end{bmatrix} - \begin{bmatrix} 8 \cdot 0 & -2 \cdot 1 \\ 4 \cdot 1^2 - 1 & 8 \cdot 0 \cdot 1 \end{bmatrix}^{-1} \begin{bmatrix} f_1(0,1) \\ f_2(0,1) \end{bmatrix} \end{aligned}$$

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$$= \begin{bmatrix} 0 \\ 1 \end{bmatrix} - \begin{bmatrix} 0 & -2 \\ 3 & 0 \end{bmatrix}^{-1} \begin{bmatrix} -1 \\ -1 \end{bmatrix}$$

§2.5 Newton's Method for System of Equations

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$$= \begin{bmatrix} 0 \\ 1 \end{bmatrix} - \begin{bmatrix} 0 & 1/3 \\ -1/2 & 0 \end{bmatrix} \begin{bmatrix} -1 \\ -1 \end{bmatrix}$$

§2.5 Newton's Method for System of Equations

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thus the first iteration gives

$$\begin{bmatrix} x_1^{(2)} \\ x_2^{(2)} \end{bmatrix} = \begin{bmatrix} 1/3 \\ 1/2 \end{bmatrix} + \begin{bmatrix} h_1^{(1)} \\ h_2^{(1)} \end{bmatrix}$$

$$= \begin{bmatrix} 1/3 \\ 1/2 \end{bmatrix} - \begin{bmatrix} 8\cdot 1/3 & -2\cdot 1/2 \\ 4\cdot(1/2)^2 - 1 & 8\cdot 1/3\cdot 1/2 \end{bmatrix}^{-1} \begin{bmatrix} f_1(1/3,1/2) \\ f_2(1/3,1/2) \end{bmatrix}$$

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thus the first iteration gives

$$\begin{bmatrix} x_1^{(2)} \\ x_2^{(2)} \end{bmatrix} = \begin{bmatrix} 1/3 \\ 1/2 \end{bmatrix} + \begin{bmatrix} h_1^{(1)} \\ h_2^{(1)} \end{bmatrix}$$

$$= \begin{bmatrix} 0.541\bar{6} \\ 1.25 \end{bmatrix}$$

§2.5 Newton's Method for System of Equations

- In general, we can use Newton's method for $F(X) = \mathbf{0}$, where $X = (x_1, x_2, \ldots, x_n)^\top$ and $F = (f_1, f_2, \ldots, f_n)^\top$.
- For higher dimensional problem, the first derivative is defined as a matrix (the **Jacobian matrix**)

$$DF(X) := \begin{bmatrix} \dfrac{\partial f_1(X)}{\partial x_1} & \dfrac{\partial f_1(X)}{\partial x_2} & \cdots & \dfrac{\partial f_1(X)}{\partial x_n} \\ \dfrac{\partial f_2(X)}{\partial x_1} & \dfrac{\partial f_2(X)}{\partial x_2} & \cdots & \dfrac{\partial f_2(X)}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\partial f_n(X)}{\partial x_1} & \dfrac{\partial f_n(X)}{\partial x_2} & \cdots & \dfrac{\partial f_n(X)}{\partial x_n} \end{bmatrix}_{n\times n}.$$

§2.5 Newton's Method for System of Equations

Newton's method: given $X^{(0)} = [x_1^{(0)}, \cdots, x_n^{(0)}]^\top$, define

$$X^{(k+1)} = X^{(k)} + H^{(k)},$$

where

$$DF(X^{(k)})H^{(k)} = -F(X^{(k)}),$$

which requires solving a large linear system at every iteration.

- vector operations: not expensive.
- function evaluations: can be expensive.
- compute the Jacobian: can be expensive.
- solving matrix equations (linear system): very expensive!

§2.5 Newton's Method for System of Equations

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- solving matrix equations (linear system): very expensive!

§2.5 Newton's Method for System of Equations

Computer project: write the computer code of Newton's method for solving the system of equations

$$\begin{cases} 3x - \cos(yz) - \dfrac{1}{2} = 0\,, \\ x^2 - 81(y+0.1)^2 + \sin(z) + 1.06 = 0\,, \\ e^{-xy} + 20z + \dfrac{10\pi - 3}{3} = 0\,, \end{cases}$$

with initial guess $(x, y, z)^\top = (0.1, 0.1, -0.1)^\top$.