

# MA 3021: Numerical Analysis I

## Solutions of Nonlinear Equations



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## Introduction

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- **A nonlinear equation:**

Let  $f : \emptyset \neq A \subseteq \mathbb{R} \rightarrow \mathbb{R}$  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  $f(x)$ .

- **A system of nonlinear equations:**

Let  $F : \emptyset \neq A \subseteq \mathbb{R}^n \rightarrow \mathbb{R}^n$  be a nonlinear vector-valued function in a vector variable  $X = (x_1, x_2, \dots, x_n)^\top$ . We are interested in finding the roots (solutions) of the equation  $F(X) = \mathbf{0}$ , i.e., **zeros of the function  $F(X)$** .

## Examples

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- 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....**
  - The third function has **no real zeros** at all.
- Matlab: `p = [1 -12 47 -60 0]; r = roots(p)`

## Objectives

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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  $x_1, \dots$ , in the end we hope that  $\lim_{n \rightarrow \infty} x_n = x^*$ .
- **Iterative methods**:
  - bisection method;
  - fixed-point method;
  - Newton's method;
  - secant method.

## Bisection method

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- **Bolzano's Theorem:**  $f \in C[a, b]$  and  $f(a)f(b) < 0 \implies \exists p \in (a, b)$  such that  $f(p) = 0$ .
- **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  $f(p_1) = 0 \implies p = p_1$ ;  
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,  $p_1 \curvearrowright p_2 \curvearrowright p_3 \curvearrowright \cdots \curvearrowright p$ .

## The bisection algorithm

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**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  $i \leq N_0$  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.

## Stopping criteria

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Let  $\varepsilon > 0$  be a given tolerance.

- $|p_N - p_{N-1}| < \varepsilon$  (Note that  $|p_N - p_{N-1}| = \frac{1}{4}|b_{N-1} - a_{N-1}|$ );
- $\frac{|p_N - p_{N-1}|}{|p_N|} < \varepsilon$ , if  $p_N \neq 0$ ;
- $|f(p_N)| < \varepsilon$

## Example

Find a root of  $f(x) = x^3 + 4x^2 - 10$ . Note that  $f(1) = -5, f(2) = 14$ . Therefore,  $\exists$  root  $p \in [1, 2]$ . Actual root is  $p = 1.365230013\dots$   
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
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
13	1.364990234375	1.365234375000	1.365112304687	-0.001943659010
14	1.365112304687	1.365234375000	1.365173339843	-0.000935847281
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
18	1.365226745605	1.365234375000	1.365230560302	0.000009030992

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



## Properties of the bisection method

- **Drawbacks:** often slow; a good intermediate approximation may be discarded; doesn't work for higher dimensional problems:  $F(X) = 0$ .
- **Advantage:** it always converges to a solution if a suitable initial interval can be chosen.
- **Theorem:**  $f \in C[a, b], f(a)f(b) < 0, f(p) = 0$ . The bisection method generates  $\{p_n\}$  with  $|p_n - p| \leq \frac{1}{2^n}(b - a), \forall n \geq 1$ .

*Proof:*

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

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

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

- **Note:**  $\therefore |p_n - p| \leq \frac{1}{2^n}(b - a) \quad \therefore p_n = p + O\left(\frac{1}{2^n}\right)$ .

## Fixed points

- $X \subseteq \mathbb{R}$ ,  $g : X \rightarrow \mathbb{R}$ . If  $p \in X$  and  $g(p) = p$ , then  $p$  is called a **fixed point of  $g$** .
- 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

$$g(x) := x - f(x), h(x) := x - \frac{f(x)}{f'(x)}, \text{ etc.}$$

- If  $p$  is a fixed point of  $g(x)$ , i.e.,  $g(p) = p$ , then  $p$  is a root of  $f(x) := x - g(x)$ ,  $h(x) := 3x - 3g(x)$ , etc.

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

- **Example:**  $g(x) = x^2 - 2$ ,  $x \in [-2, 3]$ .

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

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

## A fixed point theorem

- If  $g \in C[a, b]$  and  $g(x) \in [a, b], \forall x \in [a, b]$ , then  $g$  has a fixed point in  $[a, b]$ , i.e.,  $\exists p \in [a, b]$  s.t.  $g(p) = p$ .
- If, in addition,  $g'$  exists on  $(a, b)$  and  $\exists 0 < k < 1$  such that  $|g'(x)| \leq k, \forall x \in (a, b)$ , then the fixed point is unique in  $[a, b]$ .
- Then, for any  $p_0 \in [a, b]$  and  $p_n := g(p_{n-1}), n \geq 1$ , the sequence  $\{p_n\}$  converges to the unique fixed point  $p \in [a, b]$  and
  - $|p_n - p| \leq k^n \max\{p_0 - a, b - p_0\}, \forall n \geq 1;$
  - $|p_n - p| \leq \frac{k^n}{1-k} |p_1 - p_0|, \forall n \geq 1.$

*Proof:*

- If  $g(a) = a$  or  $g(b) = b$  then  $g$  has a fixed point in  $[a, b]$ . Suppose not, then  $a < g(a) \leq b$  and  $a \leq g(b) < b$ . 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,  $\exists p \in (a, b)$  such that  $h(p) = 0$ , i.e.,  $g(p) = p$ .
- Suppose that  $\exists p < q \in [a, b]$  are fixed points of  $g$ . Then  $g(p) = p$  and  $g(q) = q$ . By the Mean Value Theorem,  $\exists \xi \in (p, q)$  such that  $\frac{g(q) - g(p)}{q - p} = g'(\xi) \implies \frac{|g(q) - g(p)|}{|q - p|} = |g'(\xi)| \leq k < 1 \implies 1 = \frac{|q - p|}{|q - p|} \leq k < 1$ . This is a contradiction. Therefore, the fixed point is unique.

## Proof (continued)

- For  $n \geq 1$ , by the Mean Value Theorem,  $\exists \xi \in (a, b)$  such that
$$0 \leq |p_n - p| = |g(p_{n-1}) - g(p)| = |g'(\xi)| |p_{n-1} - p| \leq k |p_{n-1} - p|.$$
$$\implies 0 \leq |p_n - p| \leq k |p_{n-1} - p| \leq k^2 |p_{n-2} - p| \leq \cdots \leq k^n |p_0 - p|.$$
$$\implies \lim_{n \rightarrow \infty} |p_n - p| = 0 \Leftrightarrow \lim_{n \rightarrow \infty} p_n - p = 0 \Leftrightarrow \lim_{n \rightarrow \infty} p_n = p.$$

- $\therefore |p_n - p| \leq k^n |p_0 - p|$  and  $p \in [a, b]$ .
- $\therefore |p_n - p| \leq k^n \max\{p_0 - a, b - p_0\}, \forall n \geq 1.$

- For  $n \geq 1$ ,

$$|p_{n+1} - p_n| = |g(p_n) - g(p_{n-1})| \leq k |p_n - p_{n-1}| \leq \cdots \leq k^n |p_1 - p_0|.$$

$\therefore$  For  $m > n \geq 1$ , we have

$$\begin{aligned} |p_m - p_n| &= |p_m - p_{m-1} + p_{m-1} - p_{m-2} + \cdots + p_{n+1} - p_n| \\ &\leq |p_m - p_{m-1}| + |p_{m-1} - p_{m-2}| + \cdots + |p_{n+1} - p_n| \\ &\leq k^{m-1} |p_1 - p_0| + k^{m-2} |p_1 - p_0| + \cdots + k^n |p_1 - p_0| \\ &= k^n (1 + k + \cdots + k^{m-n-1}) |p_1 - p_0|. \end{aligned}$$

$\therefore \lim_{n \rightarrow \infty} p_n = p.$

$$\therefore |p - p_n| = \lim_{m \rightarrow \infty} |p_m - p_n| \leq k^n |p_1 - p_0| \sum_{i=0}^{\infty} k^i = k^n |p_1 - p_0| \frac{1}{1-k}.$$

( $\therefore$  geometric series with  $0 < k < 1$ )

$$\therefore |p - p_n| \leq \frac{k^n}{1-k} |p_1 - p_0|.$$

## Fixed-point iterations

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- Fixed point iterations:

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

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

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

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

- **Example:**  $f(x) = x^3 + 4x^2 - 10 = 0$  has a unique root in  $[1, 2]$ .

$$\therefore f(1) = -5 < 0, f(2) = 14 > 0,$$

$$\text{and } f'(x) = 3x^2 + 8x > 0, \forall x \in (1, 2).$$

$\therefore f$  is increasing on  $[1, 2]$ .

$\therefore f$  has a unique root in  $[1, 2]$ .

## Fixed-point problem

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root-finding problem  $\iff$  fixed-point problem.

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

## Numerical results

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Using the fixed-point iterations, we have

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

The actual root is  $p = 1.365230013\dots$

**Computer project 1:** write the Matlab files for (c), (d), and (e).

## Newton's method

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- **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

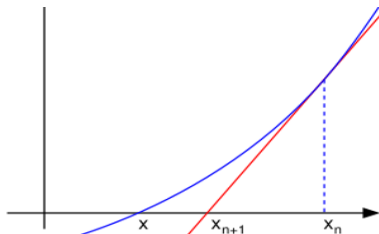
$$p \approx p_1 := p_0 - \frac{f(p_0)}{f'(p_0)}, \quad \text{provided } f'(p_0) \neq 0.$$

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

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



## 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  $p_n$  is a better approximation than  $p_{n-1}$  for the root  $p$  of the function  $f$ .
- What is the geometrical meaning of  $f'(p_{n-1}) = 0$ ?

## Example

- Consider the function  $f(x) = \cos(x) - x \Rightarrow f'(x) = -\sin(x) - 1$ .

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

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

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

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

- 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

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

## Convergence Theorem

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

*Proof:* Define  $g(x) = x - \frac{f(x)}{f'(x)}$ . Then  $g(p) = p$ .

Let  $k \in (0, 1)$ . We want to find  $\delta > 0$  s.t.

$g([p - \delta, p + \delta]) \subseteq [p - \delta, p + \delta]$  and  $|g'(x)| \leq k, \forall x \in (p - \delta, p + \delta)$ .

$\because f'(p) \neq 0$  and  $f'$  is continuous on  $[a, b]$ .

$\therefore$  By the sign-preserving property,  $\exists \delta_1 > 0$  s.t.  $f'(x) \neq 0$

$\forall x \in [p - \delta_1, p + \delta_1]$ .

$\therefore g$  is continuous on  $[p - \delta_1, p + \delta_1]$  and

$$g'(x) = 1 - \left\{ \frac{f'(x)f'(x) - f(x)f''(x)}{(f'(x))^2} \right\} = \frac{f(x)f''(x)}{(f'(x))^2}, \forall x \in [p - \delta_1, p + \delta_1].$$

$\because f \in C^2[a, b]. \quad \therefore g \in C^1[p - \delta_1, p + \delta_1].$

$\because f(p) = 0 \quad \therefore g'(p) = 0.$

$\because g'$  is continuous on  $[p - \delta_1, p + \delta_1]$ .

$\therefore \exists \delta > 0$  and  $\delta < \delta_1$  s.t.  $|g'(x)| \leq k, \forall x \in [p - \delta, p + \delta]$ .

## Convergence Theorem (continued)

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**Claim:**  $g([p - \delta, p + \delta]) \subseteq [p - \delta, p + \delta]$ .

Let  $x \in [p - \delta, p + \delta]$ .

By the MVT,  $\exists \xi$  between  $x$  and  $p$  s.t.  $|g(x) - g(p)| \leq |g'(\xi)||x - p|$ .

$\therefore |g(x) - p| \leq k|x - p| < |x - p| \leq \delta$ .

That is,  $g(x) \in [p - \delta, p + \delta]$ .

## Convergence order

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- **Definition:** Suppose  $\{p_n\}$  converges to  $p$  ( $\lim_{n \rightarrow \infty} p_n = p$ ) with  $p_n \neq p, \forall n$ . If  $\exists \lambda, \alpha > 0$  s.t.  $\lim_{n \rightarrow \infty} \frac{|p_{n+1} - p|}{|p_n - p|^\alpha} = \lambda$ , then we say that  $\{p_n\}$  converges to  $p$  of order  $\alpha$  with asymptotic error constant  $\lambda$ .
- **Note:** If  $\alpha = 1$  (and  $\lambda < 1$ ), then we say  $\{p_n\}$  is linearly convergent. If  $\alpha = 2$ , then we say  $\{p_n\}$  is quadratically convergent.

## Newton's method is quadratically convergent when it converges

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### Sketch of the proof:

$f \in C^2[a, b], f(p) = 0$ . By Taylor's Theorem, we have

$$\begin{aligned}f(x) &= f(p_n) + f'(p_n)(x - p_n) + \frac{f''(\xi)}{2!}(x - p_n)^2 \\ \implies 0 &= f(p) = f(p_n) + f'(p_n)(p - p_n) + \frac{f''(\xi)}{2!}(p - p_n)^2 \\ \implies (p - p_n) + \frac{f(p_n)}{f'(p_n)} &= -\frac{f''(\xi)}{2f'(p_n)}(p - p_n)^2 \\ \implies p - \left(p_n - \frac{f(p_n)}{f'(p_n)}\right) &= -\frac{f''(\xi)}{2f'(p_n)}(p - p_n)^2 \\ \implies |p - p_{n+1}| &\leq \frac{M}{2|f'(p_n)|} |p - p_n|^2, \quad n \geq 0 \\ &\text{(by the Extreme Value Theorem)}\end{aligned}$$

## Some remarks on Newton's method

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### Advantages:

- The convergence is **quadratic**.
- Newton's method works for higher dimensional problems.

### Disadvantages:

- Newton's method converges only **locally**; i.e., the initial guess  $p_0$  has to be close enough to the solution  $p$ .
- It needs the first derivative of  $f(x)$ .

## 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  $n \geq 2$ ,
  - compute  $a = \frac{f(p_{n-1}) - f(p_{n-2})}{p_{n-1} - p_{n-2}}$ , if  $p_{n-1} \neq p_{n-2}$ .
  - compute  $p_n = p_{n-1} - \frac{f(p_{n-1})}{a}$ , if  $f(p_{n-1}) \neq f(p_{n-2})$ .
- **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

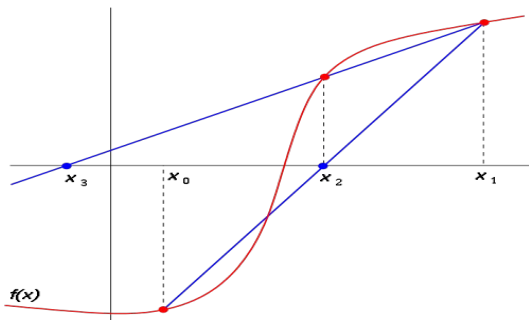
$$\lim_{n \rightarrow \infty} \frac{|p_{n+1} - p|}{|p_n - p|^{(1+\sqrt{5})/2}} = C, \quad (1 + \sqrt{5})/2 \approx 1.62 < 2.$$



## Geometrical interpretation of the secant method

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The first two iterations of the secant method. The red curve shows the function  $f$  and the blue lines are the secants.



This picture is quoted from <http://en.wikipedia.org/wiki/>

## Example

- Consider the function  $f(x) = \cos(x) - x$ .  $\exists p \in (0, \pi/2)$  such that  $f(p) = 0$ . Let  $p_0 = 0.5$  and  $p_1 = \pi/4$ .

### The secant method:

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

- Numerical results:**

$n$	$p_n$	$f(p_n)$
0	0.500000000000000	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

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

## Newton's method for systems of 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

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

- Putting it into the matrix form, we have

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

## Newton's method for systems of nonlinear equations (cont.)

- To simplify the notation we introduce the **Jacobian matrix**:

$$J(x_1, x_2) = \begin{bmatrix} \frac{\partial f_1(x_1, x_2)}{\partial x_1} & \frac{\partial f_1(x_1, x_2)}{\partial x_2} \\ \frac{\partial f_2(x_1, x_2)}{\partial x_1} & \frac{\partial f_2(x_1, x_2)}{\partial x_2} \end{bmatrix}.$$

- Then we have

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} f_1(x_1, x_2) \\ f_2(x_1, x_2) \end{bmatrix} + J(x_1, x_2) \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}.$$

- If  $J(x_1, x_2)$  is nonsingular then we can solve for  $[h_1, h_2]^T$ :

$$J(x_1, x_2) \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} = - \begin{bmatrix} f_1(x_1, x_2) \\ f_2(x_1, x_2) \end{bmatrix}.$$

## Newton's method for systems of nonlinear equations (cont.)

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

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

with

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

- 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):

$$\begin{cases} 4x_1^2 - x_2^2 = 0, \\ 4x_1x_2^2 - x_1 = 1. \end{cases}$$

## Newton's method for higher dimensional problems

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

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

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

## Operations involved in Newton's method

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

**Computer project 2:** write the computer code of Newton's method for solving the system of equations

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

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