MA 1018: Introduction to Scientific Computing
Solutions of Nonlinear Equations

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Introduction

- **A nonlinear equation:**

  Let $f : \varnothing \neq A \subseteq \mathbb{R} \to \mathbb{R}$ 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 $f(x)$.*

- **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 $F(X)$.*

Examples

- 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)`
- The n roots of a polynomial of degree n depend continuously on the coefficients. (see Complex Analysis)

  However, the problem of approximating the roots given the coefficients is ill-conditioned, see Wilkinson's polynomial.

  https://en.wikipedia.org/wiki/Wilkinson%27s_polynomial

Objectives

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 taking an initial guess x_0, then a better guess $x_1, \cdots$, in the end we hope that $\lim_{n\to\infty} x_n = x^*$.
- **Iterative methods:**
  - bisection method
  - fixed-point method
  - Newton's method
  - secant method

Bisection method

- **Bolzano's Theorem:** $f \in C[a,b]$ and $f(a)f(b) < 0 \Longrightarrow \exists\, p \in (a,b)$ 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 $f(p_1) = 0 \Longrightarrow p = p_1$;
    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 $b_2 = p_1$;
  - $p_2 = \dfrac{1}{2}(a_2 + b_2)$.
  - 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, $p_1 \to p_2 \to p_3 \to \cdots \to p$.

The bisection algorithm

Input: a, b, tolerance TOL, maximum number of iterations N_0.

Output: approximate solution of p or message of failure.

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

Step 2: while $i \le N_0$ 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

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 $p = 1.365230013...$
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`

Properties of the bisection method

- **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.
- **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 $p \in (a_n, b_n)$.

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

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

Fixed points (固定點)

- **Definition:** $X \subseteq \mathbb{R}$, $g : X \to \mathbb{R}$. 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 $g(x) := x - f(x)$, $h(x) := x - \dfrac{f(x)}{f'(x)}$, 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) $\Longleftrightarrow$ (fixed-point problem).
- **Example:** $g(x) = x^2 - 2$, $x \in [-2, 3]$.

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

  $\therefore -1$ and 2 are fixed points of function 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 $|g'(x)| \le k, \forall\, x \in (a,b)$, then the fixed point is unique in $[a,b]$.
- Then, for any $p_0 \in [a,b]$ and $p_n := g(p_{n-1}), n \ge 1$, the sequence $\{p_n\}$ converges to the unique fixed point $p \in [a,b]$ and
  - $|p_n - p| \le k^n \max\{p_0 - a, b - p_0\}, \forall\, n \ge 1$;
  - $|p_n - p| \le \frac{k^n}{1-k}|p_1 - p_0|, \forall\, n \ge 1$.

Proof:

- If $g(a) = a$ or $g(b) = b$ then g has a fixed point in $[a,b]$. Suppose not, then $a < g(a) \le b$ and $a \le g(b) < b$. 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 $\frac{g(q)-g(p)}{q-p} = g'(\xi) \Longrightarrow$ $\frac{|g(q)-g(p)|}{|q-p|} = |g'(\xi)| \le k < 1 \Longrightarrow 1 = \frac{|q-p|}{|q-p|} \le k < 1$. This is a contradiction. Therefore, the fixed point is unique.

Proof of the fixed point theorem (cont'd)

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

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

$\because \lim_{n\to\infty} p_n = p$.

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

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

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

This completes the proof. $\square$

Fixed-point iterations

- 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

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

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

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

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

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 problems

root-finding problem $\Longleftrightarrow$ 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

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	1.03×10^8				1.365230013
			$\vdots$	$\vdots$	
15			1.365223680	1.365230013	
			$\vdots$		
30			1.365230013		

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

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

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

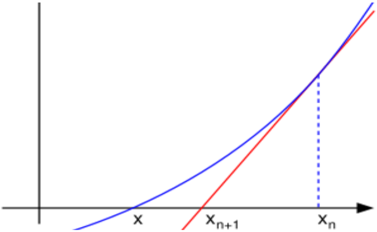
$$p \approx p_1 := p_0 - \frac{f(p_0)}{f'(p_0)}, \quad \text{provided } f'(p_0) \neq 0.$$

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

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

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

  $\because f(\pi/2) = -\pi/2 < 0$ and $f(0) = 1 > 0$.
  $\therefore \exists\, p \in (0, \pi/2)$ such that $f(p) = 0$.

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

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

- 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 $g(x) = x - \dfrac{f(x)}{f'(x)}$. Then $g(p) = p$. Let $k \in (0,1)$.

By the fixed point theorem on p. 11, we want to find $\delta > 0$ such that

$g([p-\delta, p+\delta]) \subseteq [p-\delta, p+\delta]$ 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, $\exists\, \delta_1 > 0$ such that $f'(x) \neq 0$ $\forall\, x \in [p-\delta_1, p+\delta_1]$.

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

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

Convergence Theorem (cont'd)

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

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

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

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

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. $|g(x) - g(p)| \le |g'(\xi)||x-p|$.

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

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

Convergence order

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

Sketch of the proof:

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

$$f(x) = f(p_n) + f'(p_n)(x - p_n) + \frac{f''(\xi)}{2!}(x - p_n)^2$$

$$\Longrightarrow 0 = f(p) = f(p_n) + f'(p_n)(p - p_n) + \frac{f''(\xi)}{2!}(p - p_n)^2$$

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

$$\Longrightarrow p - \left(p_n - \frac{f(p_n)}{f'(p_n)}\right) = -\frac{f''(\xi)}{2f'(p_n)}(p - p_n)^2$$

$$\Longrightarrow |p - p_{n+1}| \leq \frac{M}{2|f'(p_n)|}|p - p_n|^2, \quad n \geq 0$$

(by the Extreme Value Theorem)

Remarks on Newton's method

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 $f(x)$.

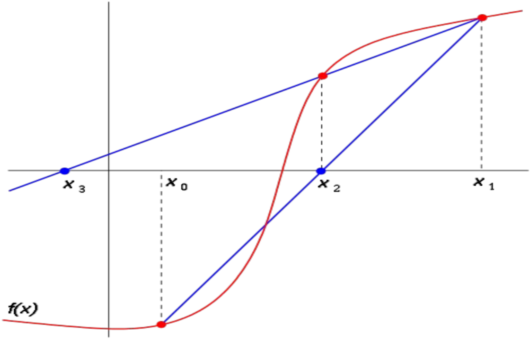
Secant method

- **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

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

Geometrical interpretation of the secant method

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
https://en.wikipedia.org/wiki/Secant_method

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	0.50000000000000	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

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'd)

- 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 $[h_1, h_2]^\top$:

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

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

- Newton's method for the system of 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

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

- **Example:**

  Use Newton's method with initial guess $\mathbf{x}^{(0)} = (0, 1)^\top$ to solve the following nonlinear system (perform two iterations):

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

Newton's method for higher dimensional problems

- In general, we can use Newton's method for $F(X) = \mathbf{0}$, where $X = (x_1, x_2, \ldots, x_n)^\top$ 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)

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

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

Operations involved in Newton's method

Operations involved in Newton's method:

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

Homework: 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 $(x, y, z)^\top = (0.1, 0.1, -0.1)^\top$.