2月27日作业

1

1. The Lambert W-function, $y = W(x)$, is the inverse function of $x = y\exp(y)$ for $y \in [-1, +\infty)$. Make a plot of the Lambert W-function, with at least 100 equally spaced sampling points over x. Verify your plot using the graph of $x = y\exp(y)$.

解：W-function 不存在初等表达式，但是：

$$\frac{dx}{dy} = e^y(y+1) \geq 0 \quad (\text{仅当 } y=-1 \text{ 取等号})$$

$\Rightarrow$ $x = ye^y$ 在 $[-1, +\infty)$ 严格单调递增

$\Rightarrow$ $x = ye^y$ 存在反函数 $y = f(x)$

显然，$\mathrm{dom}(f) = [-e^{-1}, +\infty)$

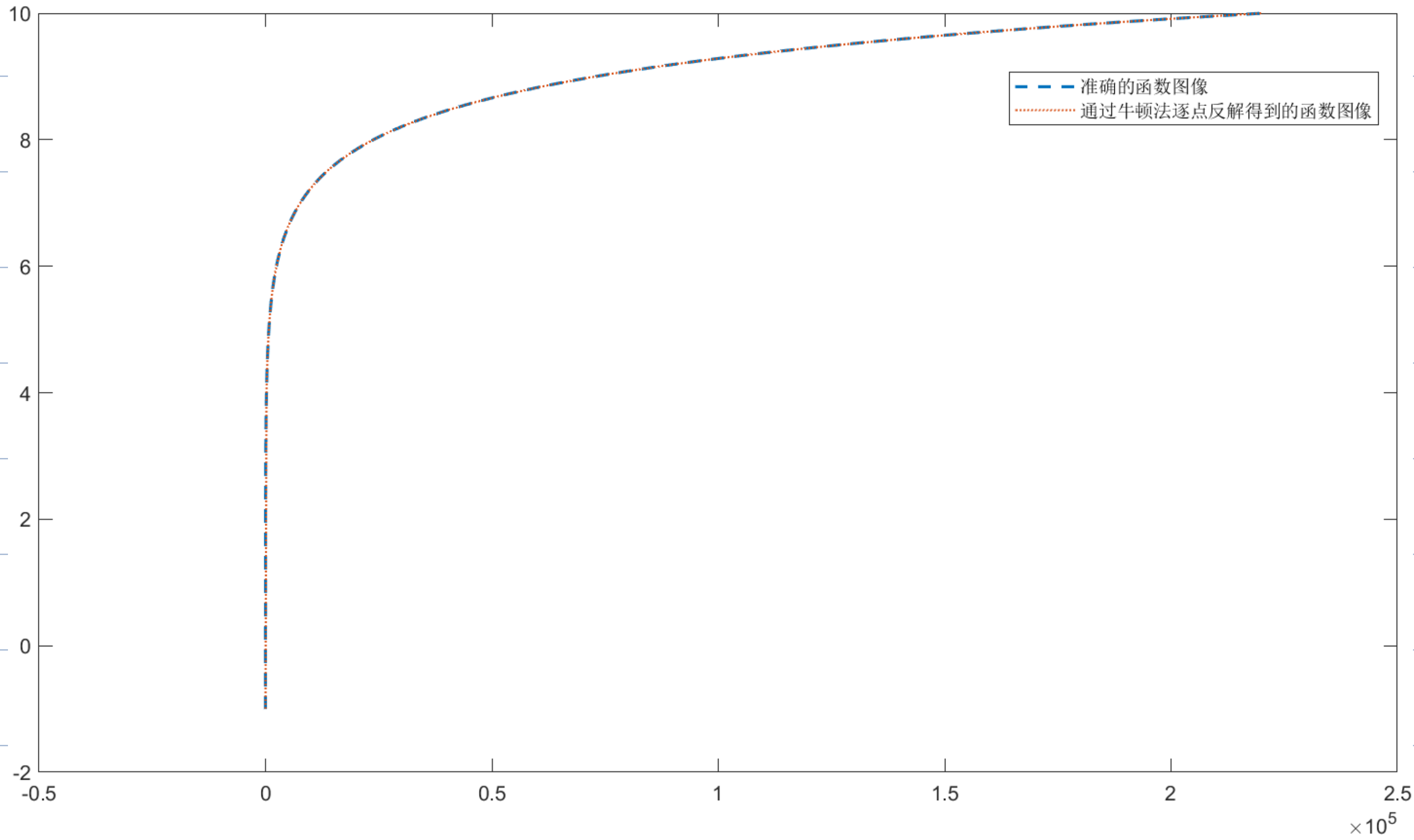
对于 $x_0 \in [-e^{-1}, +\infty)$，可以使用牛顿法求解：

$$ye^y - x_0 = 0$$

由牛顿法所得到的根 $\hat{y} \approx f(x_0)$.

(在本题中，统一对初始猜测值取 $y_0 = 10$)

以下是二者相互比较得到的图象，其中"准确的图象"指的是用 $x = y \cdot e^y$ 得到的。



可以看出，在 $x < 2.5\times10^5$ 的范围内，拟合效果很好。

2

2. Using Newton's method to find the root of $\arctan x = 0$ is an overkill, since the unique solution, $x_* = 0$, is trivial. However, this is a good example to see that the convergence of Newton's method relies on the initial guess. The set of real initial guesses such that Newton's method converges to x_* is of the form $(-\alpha, \alpha)$, where $\alpha > 0$. Try to calculate α with at least 10 significant decimal digits. What happens if α is used as the initial guess?

解：由于收敛域为 $(-\alpha, \alpha)$，并且 $y = \arctan x$ 是奇函数，

根据对称性，可以只探讨 $x_k \geq 0$ 的情况

$$x_{k+1} = x_k - \frac{\arctan x_k}{\frac{1}{1+x_k^2}} = x_k - (1+x_k^2)\arctan x_k$$

$$\Rightarrow x_{k+1} - x_k = -(1+x_k^2)\arctan x_k < 0$$

$$\Rightarrow x_{k+1} < x_k$$

令 $|x_{k+1}| \geq |x_k|$，这只可能在 $x_{k+1} < 0$ 时发生

$$|x_{k+1}| = |x_k - (1+x_k^2)\arctan x_k| \geq |x_k|$$

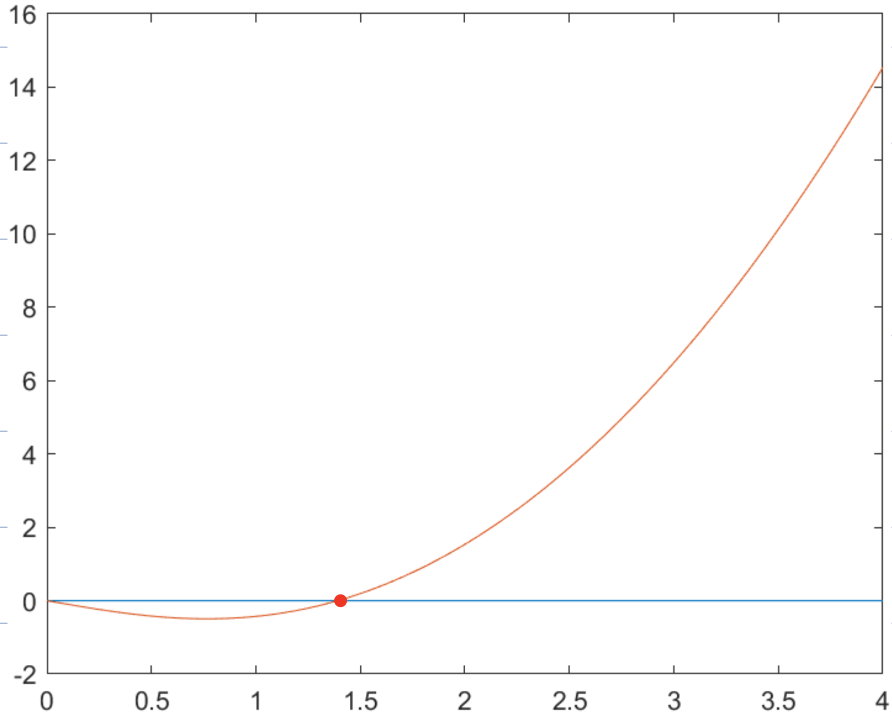
$$\Rightarrow \quad (1+x_k^2)\arctan x_k - 2x_k \geq 0$$

令 $f(x) = (1+x^2)\arctan x - 2x$

求导：$f'(x) = 1 + 2x \cdot \arctan x - 2 = 2x\arctan x - 1$

也即 $f(x)$ 先递减后递增

作出 $f(x) = (1+x^2)\arctan x - 2x$ 的图象如下：



结合 $f(0) = 0$ 可知 $f(x) = 0$ 在 $(0, +\infty)$ 只有一根

用 2 分法（见 matlab 对应文件）得到：

$$\alpha \approx 1.3917452002707$$

（14 位有效数字）

下面我将说明：当 $|x_0| \geq \alpha$ 时，不收敛，$|x_0| < \alpha$ 时，会收敛。

同样由 $y = \arctan x$ 是奇函数，可假设 $x_0 \geq 0$

① 当 $|x_0| \geq \alpha$ 时，$|x_1| \geq |x_0| \geq \alpha$

$\Rightarrow |x_2| \geq |x_1| \geq \alpha \quad \cdots \quad \Rightarrow |x_n| \geq |x_{n-1}| \geq \cdots \geq \alpha$

也即 $\{x_k\}_{k\geq 1}^{\infty}$ 不会收敛！

特别的，若 $|x_0| = \alpha$，则有 $|x_n| = |x_{n-1}| = \cdots = |x_0| = \alpha$

也即 x_k 会在 α 与 $-\alpha$ 之间来回振荡

② 若 $|x_0| < \alpha$，则有 $|x_1| < |x_0|$，$|x_2| < |x_1| \cdots$

一般的：$|x_{k+1}| < |x_k|$，即 $\{|x_k|\}_{k=1}^{\infty}$ 单调递减

显然 $|x_k| \geq 0 \Rightarrow \lim\limits_{k\to\infty} |x_k| = \beta$ 存在

假设 $\lim\limits_{k\to\infty} |x_k| = \beta > 0$

$$\lim_{k\to\infty} |x_{k+1}| = \lim_{k\to\infty} \left| x_k - (1+x_k^2)\arctan x_k \right|$$

$$\Rightarrow \quad |\beta| = |\beta - (1+\beta^2)\arctan\beta|$$

$$\Rightarrow \quad \beta = \beta - (1+\beta^2)\arctan\beta$$

或：$\beta = -\beta + (1+\beta^2)\arctan\beta$

对于第一种情况，$\beta = 0$，与假设矛盾！

对于第二种情况，由上面的讨论，必有 $\beta = \alpha$，但是 $|x_k| < \alpha$，$k = 1, 2, \cdots$ 因此也不可能成立！

因此，只能取 $\beta = 0$，即 $\lim\limits_{k\to\infty} |x_k| = 0$

即 $|x_0| < \alpha$ 时，牛顿法迭代收敛 $\square$

3

3. In this exercise, you will determine the pH of rainwater by measuring the partial pressure of carbon dioxide (CO_2). For simplicity, we suppose that the only chemical reactions in rainwater are

$$H_2O \rightleftharpoons H^+ + OH^-,$$
$$CO_2 + H_2O \rightleftharpoons H^+ + HCO_3^-,$$
$$HCO_3^- \rightleftharpoons H^+ + CO_3^{2-}.$$

The following nonlinear system of equations governs the chemistry of rainwater:

$$\begin{aligned} K_W &= [H^+][OH^-], \\ K_1 &= 10^6 \frac{[H^+][HCO_3^-]}{K_H \cdot p_{CO_2}}, \\ K_2 &= \frac{[H^+][CO_3^{2-}]}{[HCO_3^-]}, \\ [H^+] &= [OH^-] + [HCO_3^-] + 2[CO_3^{2-}], \end{aligned}$$

where $K_H = 10^{-1.46}$ is Henry's constant, and $K_1 = 10^{-6.3}$, $K_2 = 10^{-10.3}$ and $K_W = 10^{-14}$ are equilibrium constants.

Let us use $p_{CO_2} = 375$ ppm, which was the partial pressure of CO_2 at Mauna Loa (Hawaii) in 2003. Estimate the corresponding pH of rainwater.

Solve this problem using the multivariable version of Newton's method.

解：设 $x = [H^+]$, $y = [OH^-]$, $z = [HCO_3^-]$, $w = [CO_3^{2-}]$

再将各常数抽象为如下常量：

$C_1 = K_W = 10^{-14}$

$C_2 = K_1 \cdot 10^{-6} \cdot K_H \cdot P_{CO_2}$

$\quad = 10^{-6.3} \cdot 10^{-6} \cdot 10^{-1.46} \cdot 375$

$C_3 = K_2 = 10^{-10.3}$

根据各平衡方程有：

$$\begin{cases} xy - C_1 = 0 \\ xz - C_2 = 0 \\ \dfrac{xw}{z} - C_3 = 0 \\ x - y - z - 2w = 0 \end{cases}$$

若记 $v = (x, y, z, w)^T$，则有：

$$v_{k+1} = v_k - [F'(v_k)]^{-1} F(v_k) \quad \cdots\cdots (*)$$

其中：$F(v) = \begin{bmatrix} xy - c_1 \\ xz - c_2 \\ \frac{xw}{z} - c_3 \\ x-y-z-2w \end{bmatrix}$

$$F'(v) = \begin{bmatrix} y & x & 0 & 0 \\ z & 0 & x & 0 \\ \frac{w}{z} & 0 & -\frac{xw}{z^2} & \frac{x}{z} \\ 1 & -1 & -1 & -2 \end{bmatrix}$$

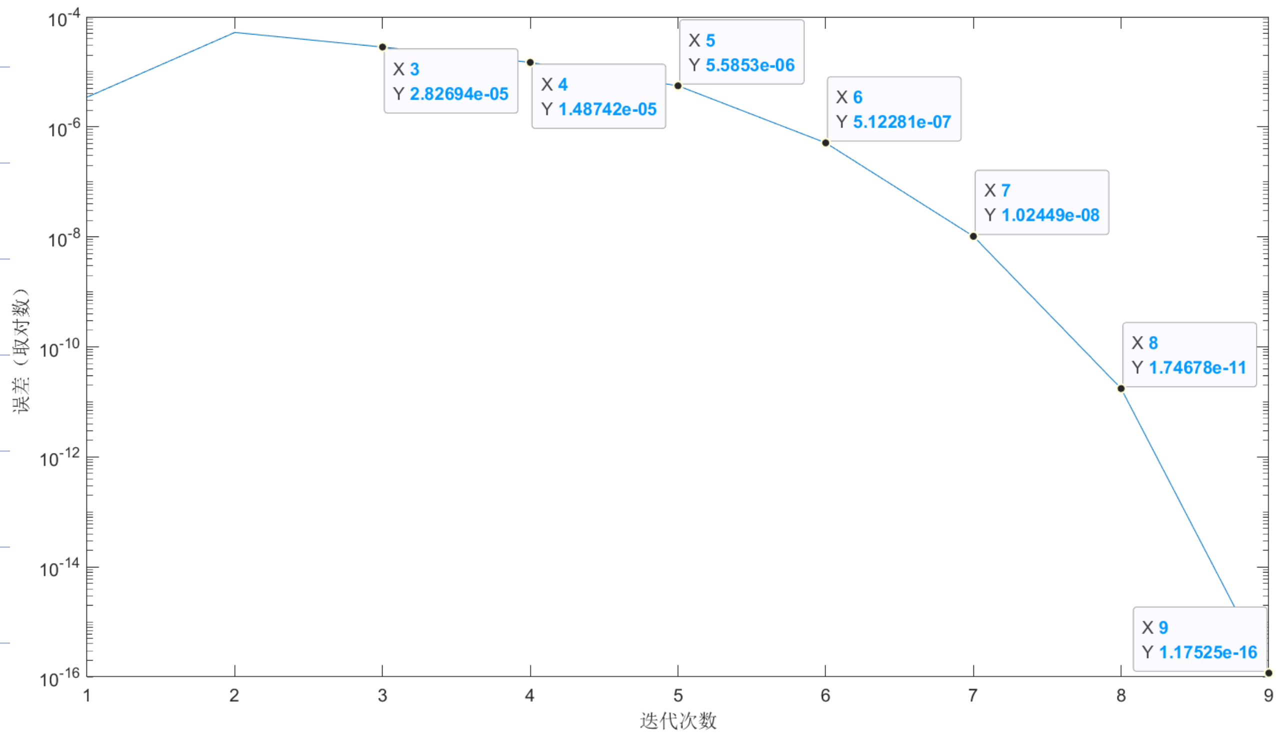
对 (*) 进行迭代，并把终止条件定为 $\|F(v_k)\|_2 \le 10^{-16}$

（具体代码详见对应 matlab 文件）

得到最后的结果为：

$pH = -\lg[H^+] \approx 5.5926$

作图：$\lg \|v_k - v_*\|_2$，观察收敛情况：

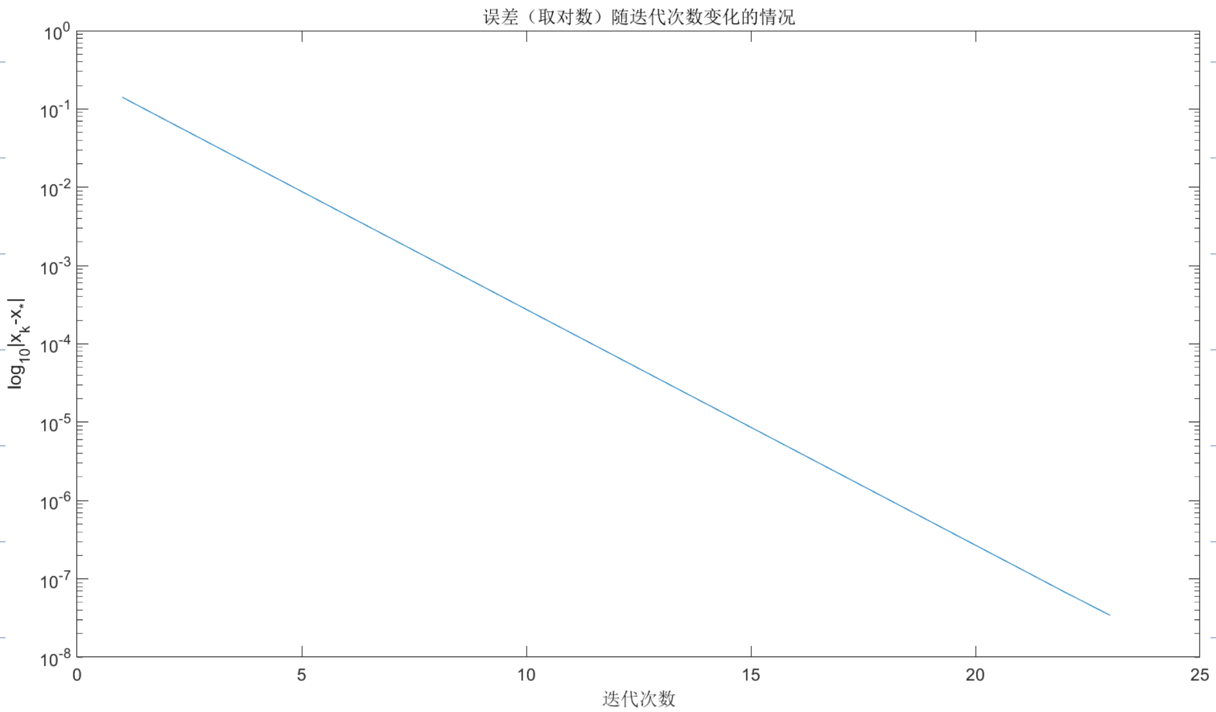


观察到 $\|V_k - V_*\|_2$ 确实有加速收敛的趋势
然而并没有发生有效数字翻倍的情况。(存疑)

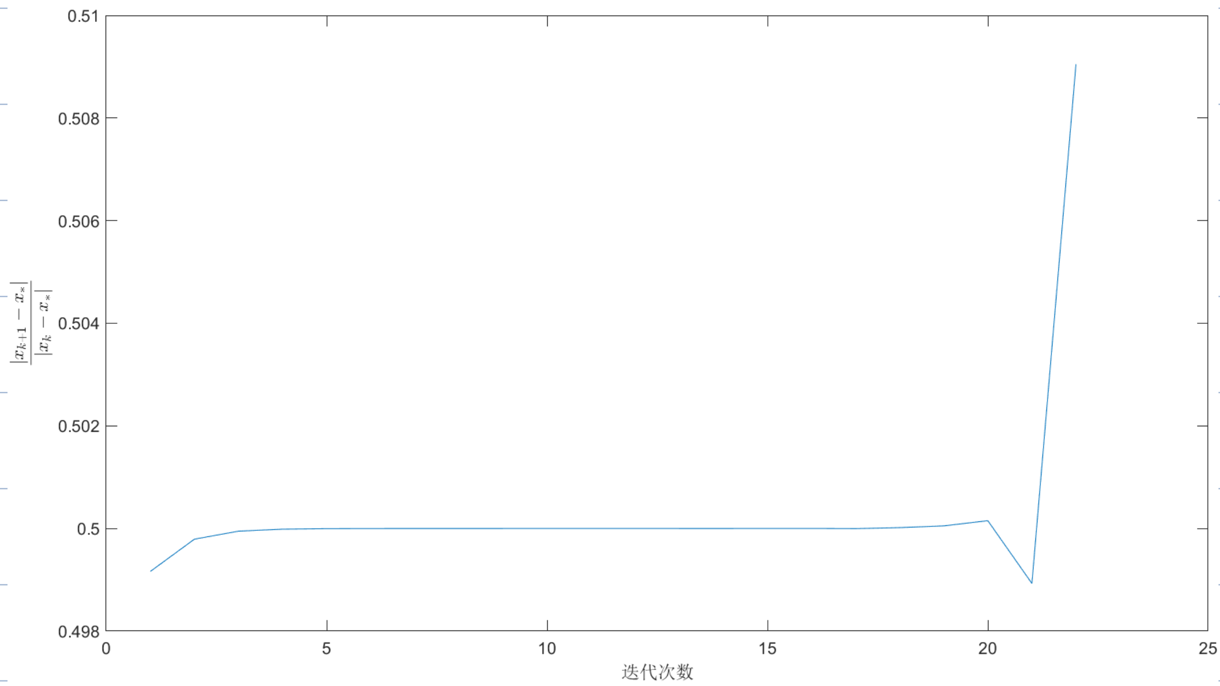
4

4. When applying Newton's method to solve the equation $f(x) = 0$, we usually require that $f'(x_*) \neq 0$, i.e., the root x_* is a simple one. Without such a condition, Newton's method is still applicable to find x_* while the convergence is no longer quadratic.
(a) Use Newton's method to solve $1 + \cos x = 0$ around $x_0 = 3$ and plot the convergence history.

(a) 使用牛顿法求解 $1+\cos x=0$ (初始值取 $x_0=3$)
对 $\log_{10}|x_k - x_*|$ 作半对数图，得到收敛过程如下：



很显然，此时牛顿法是线性收敛的。为了得到线性收敛的比例系数，我们进一步对 $\frac{|x_{k+1}-x_*|}{|x_k-x_*|}$ 作图：



定义 $e_k = |x_k - x_*|$，由上图可估计：

$$\frac{e_{k+1}}{e_k} \approx 0.5$$

(b) Let x_* be a root of $f(x)$ with multiplicity higher than one, i.e.,

$$h(x_*) = f'(x_*) = 0.$$

Show that Newton's method converges (locally) linearly around x_*.

b

设 x_* 是 $f(x)$ 的 $m+1$ 重根，即：

$$f(x_*) = f'(x_*) = \cdots = f^{(m)}(x_*) = 0 \neq f^{(m+1)}(x_*)$$

则 $f(x)$ 可以表示为：

$$f(x) = (x-x_*)^{m+1} \cdot h(x) \qquad (m \geq 0)$$

其中 $h(x_*) \neq 0$

而 $f'(x) = (m+1)(x-x_*)^m h(x) + (x-x_*)^{m+1} h'(x)$

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

$$= x_k - \frac{(x_k-x_*)^{m+1} h(x)}{(m+1)(x_k-x_*)^m h(x_k) + (x_k-x_*)^{m+1} h'(x_k)} - x_*$$

$$= (x_k - x_*) \cdot \left[1 - \frac{(x_k-x_*)^m h(x)}{(m+1)(x_k-x_*)^m h(x) + (x_k-x_*)^{m+1} h'(x_k)} \right]$$

$$= (x_k-x_*)\left[1 - \frac{1}{(m+1) + (x_k-x_*) \cdot \frac{h'(x_k)}{h(x_k)}} \right]$$

$$\Rightarrow \lim_{x_k \to x_*} \frac{|x_{k+1} - x_*|}{|x_k - x_*|} = \lim_{x_k - x_*} \left| 1 - \frac{1}{m+1 + (x_k - x_*)\frac{h'(x_k)}{h(x_k)}} \right|$$

$$= 1 - \frac{1}{m+1}$$

$$= \frac{m}{m+1}$$

因此, $m \geq 1$ 时, 牛顿法将线性收敛.

对于第(a)题而言, $m=1$, 则 $\frac{\varepsilon_{k+1}}{\varepsilon_k} \approx \frac{1}{2}$

符合理论的估计值。

c

(c) Let x_* be a root of $f(x)$ with multiplicity $m > 1$, i.e.,

$$f(x_*) = f'(x_*) = \cdots = f^{(m)}(x_*) = 0 \neq f^{(m+1)}(x_*).$$

We can modify Newton's method as

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

to achieve local quadratic convergence. Try to explain why such a modification improves the convergence.

$$x_{k+1} - x_* = x_k - \frac{(m+1)(x_k - x_*)^{m+1} h(x)}{(m+1)(x_k - x_*)^m h(x_k) + (x_k - x_*)^{m+1} h'(x_k)} - x_*$$

$$= x_k - \frac{(x_k - x_*)}{1 + \frac{(x_k - x_*)}{m+1} \cdot \frac{h'(x_k)}{h(x_k)}} - x_*$$

$$= (x_k - x_*) \cdot \left[1 - \frac{1}{1 + \frac{(x_k - x_*)}{m+1} \cdot \frac{h'(x_k)}{h(x_k)}} \right]$$

$$= (x_k - x_*) \cdot \frac{\frac{(x_k - x_*)}{m+1} \cdot \frac{h'(x_k)}{h(x_k)}}{1 + \frac{(x_k - x_*)}{m+1} \cdot \frac{h'(x_k)}{h(x_k)}}$$

$$\Rightarrow \lim_{x_k \to x_*} \frac{|x_{k+1} - x_*|}{|x_k - x_*|^2} = \lim_{x_k \to x_*} \left| \frac{\frac{h'(x_k)}{h(x_k)(m+1)}}{1 + \frac{(x_k - x_*)}{m+1} \cdot \frac{h'(x_k)}{h(x_k)}} \right|$$

$$= \left| \frac{h'(x_*)}{h(x_*) \cdot (m+1)} \right| = \text{const}$$

因此，使用改进版的牛顿法，能够做到局部二次收敛。$\square$