

(定理) A 对称正定, 则 x^* 为 $Ax = b$ 的解 的充分必要条件是:

x^* 满足 $\varphi(x^*) = \min_{x \in R^n} \varphi(x)$

$$\varphi(x) = \frac{1}{2}(Ax, x) - (b, x)$$

证明: " \Rightarrow " (3) $\Rightarrow \varphi(x) - \varphi(x^*) = \frac{1}{2}(A(x-x^*), (x-x^*)) \geq 0$
 $\varphi(x) \geq \varphi(x^*)$

" \Leftarrow " $\varphi(\bar{x}) = \min_{x \in R^n} \varphi(x) \quad \bar{x} = x^*$

(3) $\varphi(\bar{x}) - \varphi(x^*) = \frac{1}{2}(A(\bar{x} - x^*), (\bar{x} - x^*))$
 $0 \Rightarrow \bar{x} = x^* \quad \square$

$Ax = b \Leftrightarrow \exists \varphi(x)$ 最小值对应 \bar{x}

最速下降法: $y(x)$ 最小值 设 $x^{(k)}$ 已固定

给一个方向 $p^{(k)}$ 令 $x^{(k+1)} = x^{(k)} + \alpha p^{(k)}$

$$y(x^{(k+1)}) = \min_{\alpha \in \mathbb{R}} y(x^{(k)} + \alpha p^{(k)})$$

$$\frac{d y(x^{(k)} + \alpha p^{(k)})}{d \alpha} = (A(x^{(k)} + \alpha p^{(k)}) - b, p^{(k)})$$

$$\alpha_k = \frac{-(Ax^{(k)} - b, p^{(k)})}{(Ap^{(k)}, p^{(k)})}$$

$$x^{(k+1)} = x^{(k)} + \alpha_k p^{(k)}$$

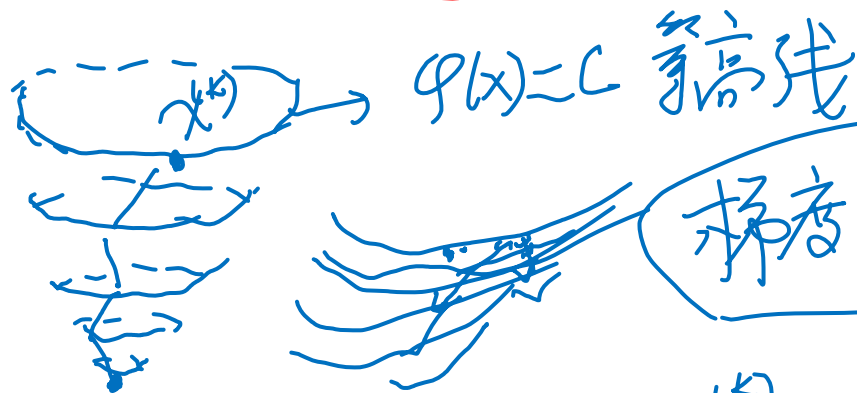
$$y(x^{(k+1)}) \leq y(x^{(k)})$$

最速下降法 (续):

$$\text{取 } p^{(k)} = -\nabla \varphi(x^{(k)}) = -(Ax^{(k)} - b) = r^{(k)} \quad (4.11)$$

$$x^{(k+1)} = x^{(k)} + \alpha_k r^{(k)} \quad \text{“最速下降法”} \quad x^{(k)} \text{ 残差}$$

且 $\lim_{k \rightarrow \infty} x^{(k)} = x^* = A^+ b$



梯度与等高线垂直

最速下降法收敛速度: $\|x^{(k)} - x^*\|_A \leq \left(\frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n} \right)^k \|x^{(0)} - x^*\|_A$

$$\|x\|_A^2 = (Ax, x)$$

$$\lambda_1 A \text{ 大 } TZZ$$

$$\lambda_n A \text{ 小 } TZZ$$

2 条件数

$$= \left(\frac{\frac{\lambda_1}{\lambda_n} - 1}{\frac{\lambda_1}{\lambda_n} + 1} \right)^k \|x^{(0)} - x^*\|_A$$

$$= \left(\frac{\text{Cond}(A) - 1}{\text{Cond}(A) + 1} \right)^k \|x^{(0)} - x^*\|_A$$

共轭梯度法:

$$\underbrace{x^{(0)} = 0}_{\text{初始值}} \quad \underbrace{p^{(0)} = r^{(0)} = b - Ax^{(0)}}_{\text{初始搜索方向}} \\ x^{(k+1)} = x^{(k)} + \alpha_k p^{(k)} \quad \text{其中 } \alpha_k \text{ 是使 } \varphi(x) \text{ 最小的值}$$

$$x^{(k)} = \alpha_0 p^{(0)} + \alpha_1 p^{(1)} + \dots + \alpha_{k-1} p^{(k-1)}$$

找 $\alpha_k, p^{(k)}$ 使 $\varphi(x^{(k)}) = \min_{x \in \text{span}\{p^{(0)}, \dots, p^{(k)}\}} \varphi(x)$

α, y

$x \in \text{span}\{p^{(0)}, \dots, p^{(k)}\}$ 分解 $x = y + \alpha p^{(k)}$

由 (2)

其中 $y \in \text{span}\{p^{(0)}, \dots, p^{(k-1)}\}$

$$\varphi(x) = \varphi(y) + \alpha (Ay, p^{(k)}) - \alpha (b, p^{(k)}) + \frac{\alpha^2}{2} (Ap^{(k)}, p^{(k)})$$

为使 $\varphi(x)$ 变为两个可独立最小化问题 令

$$(Ay, p^{(k)}) = 0 \quad \forall y \in \text{span}\{p^{(0)}, \dots, p^{(k-1)}\} \\ (Ap^{(j)}, p^{(k)}) = 0 \quad j = 0, 1, \dots, k-1$$

(定义: A-共轭向量组或A-正交向量组)

$$\left\{ \begin{array}{l} A \text{ 对称正定} \text{ 若 } p^{(0)} \dots p^{(m)} \text{ 满足} \\ (A p^{(i)}, p^{(j)}) = 0 \quad i \neq j, \quad i, j = 0, 1, \dots, m \end{array} \right.$$

称 $p^{(i)}$ 为 A 共轭向量组 A 正交向量组

$$\min_{y \in \text{span}\{p^{(0)}, \dots, p^{(k)}\}} \varphi(y) = \min_{y \in \text{span}\{p^{(0)}, \dots, p^{(k-1)}\}} \varphi(y) + \min_{\alpha} \left[\frac{\alpha^2}{2} (A p^{(k)}, p^{(k)}) - \alpha (b, p^{(k)}) \right]$$

$$x^{(k+1)} = x^{(k)}$$

$$\alpha_k = \frac{(r^{(k)}, p^{(k)})}{(A p^{(k)}, p^{(k)})}$$

$$x^{(k+1)} = x^{(k)} + \alpha_k p^{(k)}$$

共轭梯度法

774: p210. 9

$P^{(0)}, P^{(1)}, \dots, P^{(k)}$ 的选择

若 $p^{(0)} \dots p^{(k-1)}$ 已选好

$$r^{(k)} = b - Ax^{(k)}$$

如何选 $p^{(k)}$?

$$p^{(k)} = r^{(k)} + \beta_{k-1} p^{(k-1)}$$

$$\text{让 } (p^{(k)}, Ap^{(k-1)}) = 0$$

$$\Rightarrow \beta_{k-1} = - (r^{(k)}, Ap^{(k-1)}) / (p^{(k-1)}, Ap^{(k-1)})$$

A 正交?
对称?

流程: $x^{(k)} \xrightarrow{p^{(k-1)} \text{ 已知}} r^{(k)} = b - Ax^{(k)} \xrightarrow{\beta_{k-1}} p^{(k)} \xrightarrow{\alpha_k} x = x^{(k)} + \alpha_k p^{(k)}$

$$* \quad r^{(k+1)} = b - Ax^{(k+1)} = b - Ax^{(k)} - \alpha_k Ap^{(k)} = \underline{r^{(k)} - \alpha_k Ap^{(k)}}$$

$$* \quad (r^{(k+1)}, p^{(k)}) = (r^{(k)}, p^{(k)}) - \alpha_k (Ap^{(k)}, p^{(k)}) = 0$$

$$* \quad (r^{(k)}, p^{(k)}) = (r^{(k)}, r^{(k)} + \beta_{k-1} p^{(k-1)}) = (r^{(k)}, r^{(k)})$$

$$\therefore \alpha_k = (r^{(k)}, r^{(k)}) / (p^{(k)}, Ap^{(k)})$$

(定理: 双正交性)

CG法得到的 $r^{(k)}$ 与 $p^{(k)}$ 满足

$$(1) (r^{(i)}, r^{(j)}) = 0 \quad (i \neq j) \quad (2) \underbrace{(Ap^{(i)}, p^{(j)}) = 0}_{A \text{ 正交 } A \text{ 共轭}} \quad (i \neq j) \quad \text{且 } p^{(i)} \neq 0$$

证明: (若有时间)

证

证

$$\beta_k = \frac{(r^{(k+1)}, r^{(k+1)})}{(r^{(k)}, r^{(k)})}$$

证明：（若有时间）

共轭梯度法收敛速度:

$$\|x^{(k)} - x^*\|_A \leq 2$$

$$\left(\frac{\sqrt{\text{cond}(A)_2} - 1}{\sqrt{\text{cond}(A)_2} + 1} \right)^k \|x^{(0)} - x^*\|_A$$

快于
最速下降法

共轭梯度法是一种直接法。但是常用作迭代法

0 0 0

CG算法:

$$(1) \quad x^{(0)} \in \mathbb{R}^n \quad r^{(0)} = b - Ax^{(0)} \quad p^{(0)} = r^{(0)}$$

$$(2) \quad k = 0, 1, 2, \dots$$

$$\alpha_k = \frac{(r^{(k)}, r^{(k)})}{(p^{(k)}, A p^{(k)})}$$

$$x^{(k+1)} = x^{(k)} + \alpha^{(k)} p^{(k)}$$

$$r^{(k+1)} = r^{(k)} - \alpha_k A p^{(k)}$$

$$\beta_k = \frac{(r^{(k+1)}, r^{(k+1)})}{(r^{(k)}, r^{(k)})}$$

$$p^{(k+1)} = r^{(k+1)} + \beta_k p^{(k)}$$

$$(3) \quad \text{若 } \boxed{r^{(k)} = 0} \text{ 或 } (p^{(k)}, A p^{(k)}) = 0 \text{ 则停止}$$

$$A x^{(k)} - b = 0$$

$$x^{(k)} \text{ 为所求}$$

$$\Downarrow \quad p^{(k)} = 0 \Rightarrow \alpha^{(k)} = 0$$

第七章：非线性方程、方程组数值解法

1. 基本问题

(一) 问题描述与动机（方程求根、极值等）：

$f(x)=0$ 求根 $x^2-1=0 \Rightarrow x=\pm 1$ $xe^x=1$? 求根

n 次多项式 当 $n \geq 5$ 时无求根公式

求极值(最值)问题 最终也转化为求根问题

定义: $f(x)=0$ 若 x^* 满足 $f(x^*)=0$ 称 x^* 为 $f(x)=0$ 的一个根 (导数为0)

若 $f(x)=(x-x^*)^m g(x)$, $g(x^*) \neq 0$

则 x^* 为 $f(x)=0$ 的 m 重根

(二) 求根的基本步骤:

(1) 根的存在性, 有几个根

(2) 根的隔离: 把某个根的大致区间找出来

(3) 根的精确化: 设计算法求近似根, 满足一定精度

m 重根 $\Leftrightarrow f(x^*)=f'(x^*)=\dots=f^{(m-1)}(x^*)=0$
 $f^{(m)}(x^*) \neq 0$

(三) 单重根的二分法: f 在 $[a, b]$ 连续 $(f(a) \cdot f(b) < 0)$ 11:28 回来

则 f 在 (a, b) 有一根

1) $[a, b]$ 中点 $x_0 = \frac{a+b}{2}$ 若 $f(x_0) = 0$ x_0 为根 若不然 $f(x_0) \neq 0$

若 $f(x_0) \cdot f(a) < 0$ 取 $[a_1, b_1] = [a, x_0]$ 若 $f(x_0) \cdot f(b) < 0$ 取 $[a_1, b_1] = [x_0, b]$

则根在 $[a_1, b_1]$ 中 且 $b_1 - a_1 = \frac{b-a}{2}$

依次下去 $[a_n, b_n] = \begin{cases} [a_{n-1}, x_{n-1}] & \text{若 } f(x_{n-1}) \cdot f(a_{n-1}) < 0 \\ [x_{n-1}, b_{n-1}] & \text{若 } f(x_{n-1}) \cdot f(b_{n-1}) < 0 \end{cases}$

$$x_{n-1} = \frac{a_{n-1} + b_{n-1}}{2}$$

则 $x_n = \frac{a_n + b_n}{2}$ 作为 x^* 近似值 且 $|b_n - a_n| = \frac{b-a}{2^n}$ "停止"

误差与停止原则:

$$|e_n| = |x_n - x^*| \leq \frac{b-a}{2^{n+1}}$$

若要 $|e_n| < \varepsilon$ 只要 $\frac{b-a}{2^{n+1}} < \varepsilon$ 即可

$$n > \log_2 \frac{b-a}{\varepsilon} - 1$$

缺点: ①不能求偶数重根 ②收敛慢 ③不能推广到复数

2. 迭代法

（一）问题描述：

2. 迭代法
(一) 问题描述: $f(x)=0 \Leftrightarrow$ 同解 $x=y(x)$ 例

$f(x^*) = 0 \Leftrightarrow x^* = g(x^*)$ ~~此时~~ $x^* = g(x^*)$ 和 x^* 为 $g(x)$ 的不动点 _{in}

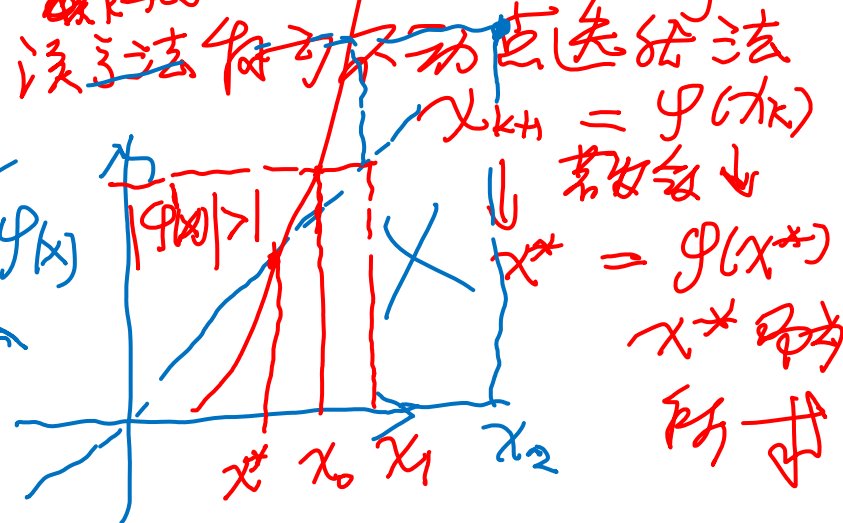
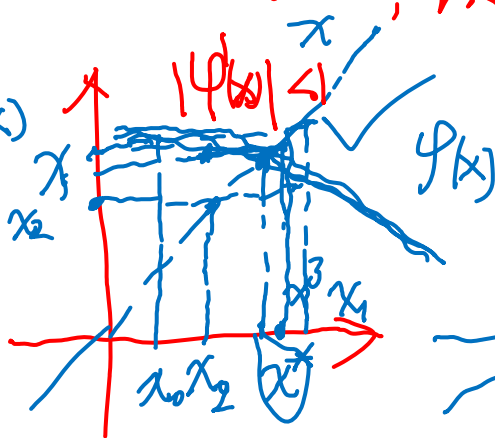
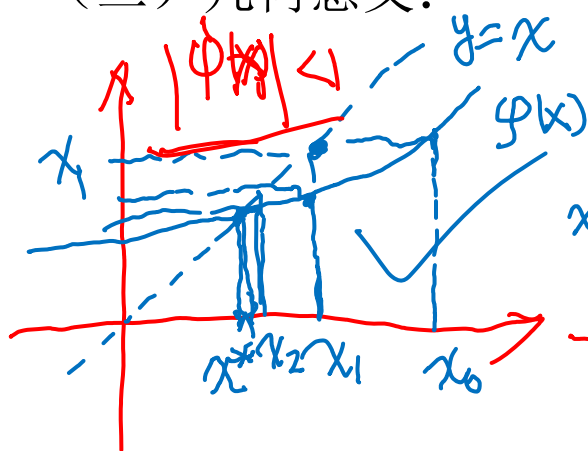
$x^3 - x - 1 = 0$ ① $x = x^3 - 1$ $g(x) = x^3 - 1$
 ② $x = \sqrt[3]{1+x}$ $g(x) = \sqrt[3]{1+x}$

更一般地 $\underline{x = x - f(x)} \quad \underline{g(x) = x - f(x)}$

(定义): 不动点迭代法 x_0 取定 $x_1 = f(x_0)$ $x_2 = f(x_1) \sim$

$$\underline{x_{k+1}} = f(x_k) \quad k=0,1,2,\dots \quad \frac{1}{n} \quad \lim_{k \rightarrow \infty} x_k = x^* \quad \text{by 8.2}$$

(二) 几何意义:



(三) 不动点存在性与迭代法的收敛性:

$$x, y \in [a, b] \quad y = \varphi(x)$$

(定理: 存在性): ① 若 $x \in [a, b]$ 时, $\varphi(x) \in [a, b]$, 且 $\varphi(x)$ 满足

② $|\varphi(x) - \varphi(y)| \leq L|x - y|, \quad L < 1, \quad x, y \in [a, b],$
则 $x = \varphi(x)$ 在 $[a, b]$ 内存在唯一的不动点 x^* .

② 压缩映射

证明: $f(x) = x - \varphi(x)$ 若 $f(a) = 0$ a 为所求
 $f(b) = 0$ b 为所求
若 $f(a) \neq 0, f(b) \neq 0$ 则 $f(a) = a - \varphi(a) < 0$ ($\varphi(a) > a$)
 $f(b) = b - \varphi(b) > 0$ ($\varphi(b) < b$)

介值定理 存在 x^* $f(x^*) = 0$ $x^* = \varphi(x^*)$

若 $x_1^* = \varphi(x_1^*) \quad x_2^* = \varphi(x_2^*)$ 则

$$|x_1^* - x_2^*| = |\varphi(x_1^*) - \varphi(x_2^*)| \leq L|x_1^* - x_2^*| \quad (L < 1)$$
$$\Rightarrow x_1^* - x_2^* = 0 \Rightarrow x_1^* = x_2^* \text{ "唯一" } \square$$

(三) 不动点存在性与迭代法的收敛性 (续):

(定理: 收敛性): 若(1) $x \in [a, b]$ 时, $\varphi(x) \in [a, b]$, 且 $\varphi(x)$ 满足

(2) $|\varphi(x) - \varphi(y)| \leq L|x - y|$, $L < 1$, $x, y \in [a, b]$

则对任何初值 x_0 , 迭代法 $x_{k+1} = \varphi(x_k)$ 都收敛于 $x = \varphi(x)$ 不动点 x^* , 并且

$$|x^* - x_k| \leq \frac{1}{1-L} |x_{k+1} - x_k|, \quad |x^* - x_k| \leq \frac{L^k}{1-L} |x_1 - x_0|$$

停止迭代 误差

$$\text{证明: (a) } x_k = \varphi(x_{k-1}) \quad x^* = \varphi(x^*) \quad \text{b) } |x_k - x^*| = |\varphi(x_{k-1}) - \varphi(x^*)| \\ \leq L |x_{k-1} - x^*| \leq L^2 |x_{k-2} - x^*| \leq \dots \leq L^k |x_0 - x^*|$$

$$\text{c) } k \rightarrow \infty \quad 0 < L < 1 \quad \lim_{k \rightarrow \infty} x_k = x^*$$

$$\text{b) } |x_k - x^*| \leq |x_k - x_{k+1}| + |x_{k+1} - x^*| \leq |x_k - x_{k+1}| + L |x_k - x^*| \\ (1-L) |x_k - x^*| \leq |x_k - x_{k+1}| \quad \checkmark$$

$$\text{c) } |x_k - x^*| \leq \frac{1}{1-L} |x_{k+1} - x_k| \leq \frac{1}{1-L} L |x_k - x_{k-1}| \leq \dots \leq \frac{L^k}{1-L} |x_1 - x_0|$$

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

(三) 不动点存在性与迭代法的收敛性 (续):

(推论: 收敛性): 前面定理中, 条件

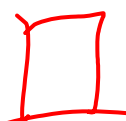
$$|\varphi(x) - \varphi(y)| \leq L|x - y|, \quad L < 1, \quad x, y \in [a, b]$$

可换成 $|\varphi'(x)| \leq L < 1, \quad x \in [a, b]$

$\xi \in (x, y)$

证明: $|\varphi(x) - \varphi(y)| = |\varphi'(\xi)(x - y)| \leq L|x - y|$

$$0 < L < 1$$



(例): 求方程 $xe^x - 1 = 0$ 在 $[0.5, \ln 2]$ 中的根

① $[a, b]$

② $|\varphi'(x)| < 1 \quad x \in [a, b]$

解: $x = e^{-x} = \varphi(x) \quad = e^{-0.5} \quad = \frac{1}{2}$

{ ① $\varphi: [a, b] \rightarrow [a, b]$ $\varphi(0.5) \quad \varphi(\ln 2)$ ✓

{ ② $|\varphi'(x)| = |e^{-x}| < 1 \quad x \in [0.5, \ln 2]$

$$x_{k+1} = \varphi(x_k) \quad \text{472}$$

(例) :

$$x^3 - x - 1 = 0 \quad \left\{ \begin{array}{l} x = x^3 - 1 = \varphi_1 \quad x \in [1, 2] \text{ 中} \\ x = \sqrt[3]{x+1} = \varphi_2 \end{array} \right.$$

$$|\varphi_2'(x)| = \left| \frac{1}{3} (x+1)^{-\frac{2}{3}} \right| \leq \frac{1}{3} \cancel{\frac{1}{3}} \frac{1}{3} 2^{-\frac{2}{3}} < 1$$

$$|\varphi_1'(x)| = |3x^2| \neq \textcircled{3} \quad x \in [1, 2]$$

~~3~~ ✓

(四) 局部收敛性:

(定义): $\varphi(x)$ 有不动点 x^* , 如果存在 x^* 的某邻域 $D: |x - x^*| < \delta$, 任意初值 $x_0 \in D$, 迭代法 $x_{k+1} = \varphi(x_k)$ 收敛于 x^* , 则称该迭代法是局部收敛的

$$D: |x - x^*| < \delta \quad x_0 \in D$$

(定理: 局部收敛性): $x = \varphi(x)$ 的不动点为 x^* , $\varphi(x)$ 在 x^* 某邻域内具有连续的一阶导数, 且 $|\varphi'(x^*)| < 1$, 则迭代法 $x_{k+1} = \varphi(x_k)$ 局部收敛

证: 存在邻域 $D: |x - x^*| < \delta$ 使 $|\varphi'(x)| < 1, x \in D$

$$\begin{aligned} \lim_{x \rightarrow x^*} \varphi'(x) &= \varphi'(x^*) \quad \forall \varepsilon > 0 \quad \exists \delta > 0 \quad |x - x^*| < \delta \Rightarrow \\ \varphi(x) &\in D \cup \{x^*\} \Rightarrow D \quad |\varphi'(x) - \varphi'(x^*)| < \varepsilon \quad \varepsilon = \varepsilon_0 = \frac{1 - |\varphi'(x^*)|}{2} \\ \therefore |\varphi'(x)| &\leq |\varphi'(x^*)| + \varepsilon \leq \frac{1 + |\varphi'(x^*)|}{2} < 1 \leq |x - x^*| \\ \text{在 } D \text{ 中 } |\varphi'(x)| &< 1 \\ \varphi(x) &\in D? \quad |\varphi(x) - x^*| = |\varphi(x) - \varphi(x^*)| \leq |\varphi'(x)| |x - x^*| \leq |x - x^*| \end{aligned}$$

(四) 局部收敛性:

(例): 求 $x^2 - 3 = 0$ 的根 $x^* = 3$

p 238. 2, 3, 4