数值算法 II 期末考试 (2025 春)

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Problem 1

给定至多 n 次的实系数多项式 $p(x) = \sum_{k=0}^{n} a_k x^k$
试分析计算 $p(x)$ 的舍入误差.

- **(舍入误差的记号)**
  n 层舍入误差 γ_n 有多种定义方法:

$$\gamma_n = \begin{cases} \frac{n\cdot\mathrm{eps}}{1-n\cdot\mathrm{eps}}, & \text{(definition 1)} \\ (1+\mathrm{eps})^n - 1, & \text{(definition 2)} \\ (1-\mathrm{eps})^{-n} - 1, & \text{(definition 3)} \end{cases}$$

  其中 eps 代表机器精度.
  第一种定义有时会过大，第二种定义最好，但并非所有场景都可使用，第三种定义是通用的.
- **(乘加运算)**
  现代硬件 (如 IEEE 754-2008 规范中的浮点单元) 引入了 **FMA** (fused multiply-add) 指令，
  以便在单个指令内精确计算 $a \cdot b + c$，中间不进行舍入，仅在最终结果舍入一次.
  这可以提高速度 (单个指令完成三元操作)，
  同时提高精度，减少误差传播 (只舍入一次，而非舍入两次):

$$\mathrm{fl}(a \cdot b + c) = (a \cdot b + c)(1+\delta) \quad (|\delta| < \mathrm{eps})$$

Solution:
考虑使用秦九韶算法计算多项式值 $p(x)$:

$$p(x) = \underbrace{x(x(\cdots x(x(x}_{n \text{ times}} a_n + a_{n-1}) + a_{n-2}) + \cdots) + a_1) + a_0$$

总共需要 n 次乘加运算 (fused multiply-add, FMA):

$$\mathrm{fl}(p(x)) = \left[\underbrace{x(x(\cdots x(x(x}_{n \text{ times}} a_n + a_{n-1}) \cdot (1+\delta_1) + a_{n-2}) \cdot (1+\delta_2) + \cdots) \cdot (1+\delta_{n-2}) + a_1) \cdot (1+\delta_{n-1}) + a_0 \right] (1+\delta_n)$$
$$\text{where } |\delta_i| < \mathrm{eps} \text{ for } i = 1, \ldots, n$$

因此我们有:

$$\begin{aligned} |\mathrm{fl}(p(x)) - p(x)| &\le \left[\underbrace{|x|(|x|(\cdots |x|(|x|(|x|}_{n \text{ times}} |a_n| + |a_{n-1}|) + |a_{n-2}|) + \cdots) + |a_1|) + |a_0| \right] \cdot \left[\prod_{k=1}^{n} (1+\delta_k) - 1 \right] \\ &= \left[\prod_{k=1}^{n} (1+\delta_k) - 1 \right] \cdot \sum_{k=0}^{n} |a_k||x|^k \\ &\lesssim [(1+\mathrm{eps})^n - 1] \cdot \sum_{k=0}^{n} |a_k||x|^k \\ &= \gamma_n \cdot \sum_{k=0}^{n} |a_k||x|^k \end{aligned}$$

Problem 2

设 f 二阶连续可导，$0 = f(x_\star) \neq f(x_\star)$，即 $x_\star$ 是 f 的单重根.
考虑 Newton 迭代格式的变体:

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

其中当 $x_k \to x_\star$ 时我们有 $\theta_k \to 0$ 成立.
请分析 θ_k 需要满足什么条件才能使上述迭代格式满足局部二次收敛性.

Solution:

$$
\begin{aligned}
x_{k+1} - x_\star &= \left(x_k - \frac{f(x_k)}{f'(x_k)+\theta_k}\right) - x_\star \\
&= (x_k - x_\star) - \frac{f(x_\star) + f'(x_\star)(x_k - x_\star) + O((x_k - x_\star)^2)}{f'(x_k)+\theta_k} \quad (\text{note that } f(x_\star)=0) \\
&= \frac{(f'(x_k)+\theta_k)(x_k - x_\star) - f'(x_\star)(x_k - x_\star) + O((x_k - x_\star)^2)}{f'(x_k)+\theta_k}
\end{aligned}
$$

当且仅当 $\theta_k = O(x_k - x_\star)$ 时 $x_{k+1} - x_\star = O((x_k - x_\star)^2)$ (即满足局部二次收敛性).

例如 **Steffensen 方法**:

$$
\begin{array}{l}
\text{Let } \theta_k = \dfrac{f(x_k + f(x_k)) - f(x_k)}{f(x_k)} - f'(x_k) \\
\hline
\begin{aligned}
x_{k+1} &= x_k - \frac{f(x_k)}{f'(x_k)+\theta_k} \\
&= x_k - \frac{f(x_k)}{f'(x_k) + \frac{f(x_k+f(x_k))-f(x_k)}{f(x_k)} - f'(x_k)} \\
&= x_k - \frac{(f(x_k))^2}{f(x_k + f(x_k)) - f(x_k)}
\end{aligned}
\end{array}
$$

注意到:

$$
\begin{aligned}
\theta_k &= \frac{f(x_k + f(x_k)) - f(x_k)}{f(x_k)} - f'(x_k) \\
&= \frac{f(x_k) + f'(x_k)f(x_k) + O((f(x_k))^2) - f(x_k)}{f(x_k)} - f'(x_k) \\
&= O(f(x_k)) \\
&\quad (\text{note that } f \text{ is a continuous function, } f(x_k) \to f(x_\star) = 0 \text{ if } x_k \to x_\star) \\
&= O(x_k - x_\star)
\end{aligned}
$$

根据前面的结论可知 Steffensen 方法具有局部二次收敛性.

事实上，Steffensen 法的收敛性分析可做得更精确.
利用 Taylor 展开可得:

$$
\begin{array}{l}
\text{Denote } \varepsilon_k := x_k - x_\star \\
\hline
\begin{aligned}
f(x_k) &= f(x_\star) + f'(x_\star)\varepsilon_k + O(\varepsilon_k^2) \\
&= f'(x_\star)\varepsilon_k + O(\varepsilon_k^2)
\end{aligned} \\
\hline
\begin{aligned}
\theta_k &= \frac{f(x_k + f(x_k)) - f(x_k)}{f(x_k)} - f'(x_k) \\
&= \frac{f(x_k) + f'(x_k)f(x_k) + \frac{f''(x_k)}{2}(f(x_k))^2 + O((f(x_k))^3) - f(x_k)}{f(x_k)} - f'(x_k) \\
&= \frac{f''(x_k)}{2} f(x_k) + O((f(x_k))^2) \\
&= \frac{f''(x_k)f'(x_\star)}{2}\varepsilon_k + O(\varepsilon_k^2)
\end{aligned} \\
\hline
\begin{aligned}
0 &= f(x_\star) \\
&= f(x_k) - f'(x_k)\varepsilon_k + \frac{f''(x_k)}{2}\varepsilon_k^2 + O(\varepsilon_k^3)
\end{aligned}
\end{array}
$$

代入 Steffensen 方法的迭代格式可得:

$$
\begin{aligned}
\varepsilon_{k+1} &= x_{k+1} - x_\star \\
&= \left(x_k - \frac{f(x_k)}{f'(x_k)+\theta_k}\right) - x_\star \\
&= \varepsilon_k - \frac{f(x_k)}{f'(x_k)+\theta_k} \\
&= \frac{f'(x_k)\varepsilon_k + \theta_k\varepsilon_k - f(x_k)}{f'(x_k)+\theta_k} \\
&= \frac{f'(x_k)\varepsilon_k + (\frac{f''(x_k)f'(x_\star)}{2}\varepsilon_k + O(\varepsilon_k^2))\varepsilon_k - f(x_k)}{f'(x_k)+O(\varepsilon_k)} \\
&= \frac{\frac{f''(x_k)f'(x_\star)}{2}\varepsilon_k^2 + \frac{f''(x_k)}{2}\varepsilon_k^2 + O(\varepsilon_k^3)}{f'(x_k)+O(\varepsilon_k)} \\
&= \frac{f''(x_k)}{2f'(x_k)}(f'(x_\star)+1)\varepsilon_k^2 + O(\varepsilon_k^3) \\
&= \frac{f''(x_\star)}{2f'(x_\star)}(f'(x_\star)+1)\varepsilon_k^2 + O(\varepsilon_k^3)
\end{aligned}
$$

因此当 $f'(x_\star)=-1$ 或 $f''(x_\star)=0$ 时，Steffensen 方法至少局部 3 次收敛.

更严格的解法:

$$
\begin{aligned}
(f(x_k))^2 &= \left(f'(x_\star)(x_k-x_\star) + \frac{f''(x_\star)}{2}(x_k-x_\star)^2 + O((x_k-x_\star)^3)\right)^2 \\
&= (f'(x_\star))^2(x_k-x_\star)^2 + f'(x_\star)f''(x_\star)(x_k-x_\star)^3 + O((x_k-x_\star)^4)
\end{aligned}
$$

$$
\begin{aligned}
f(x_k+f(x_k)) - f(x_k) &= [f(x_\star+f(x_\star)) - f(x_\star)] \\
&\quad + [f'(x_\star+f(x_\star))(1+f'(x_\star)) - f'(x_\star)](x_k-x_\star) \\
&\quad + \frac{1}{2}[f''(x_\star+f(x_\star))(1+f'(x_\star))^2 + f'(x_\star+f(x_\star))f''(x_\star) - f''(x_\star)](x_k-x_\star)^2 \\
&\quad + O((x_k-x_\star)^3) \\
&\quad (\text{note that } f(x_\star)=0) \\
&= (f'(x_\star))^2(x_k-x_\star) + \frac{1}{2}f''(x_\star)f'(x_\star)(f'(x_\star)+3)(x_k-x_\star)^2 + O((x_k-x_\star)^3)
\end{aligned}
$$

> **计算 $(f(x_k))^2$ Taylor 展开的另一种方法:**
>
> $$
> \begin{aligned}
> (f(x_k))^2 &= (f(x_\star))^2 + 2f(x_\star)f'(x_\star)(x_k-x_\star) \\
> &\quad + \frac{1}{2}\cdot 2[f(x_\star)f''(x_\star) + (f'(x_\star))^2](x_k-x_\star)^2 \\
> &\quad + \frac{1}{6}\cdot 2[f'(x_\star)f''(x_\star) + f(x_\star)f'''(x_\star) + 2f'(x_\star)f''(x_\star)](x_k-x_\star)^3 + O((x_k-x_\star)^4) \\
> &\quad (\text{note that } f(x_\star)=0) \\
> &= (f'(x_\star))^2(x_k-x_\star)^2 + f'(x_\star)f''(x_\star)(x_k-x_\star)^3 + O((x_k-x_\star)^4)
> \end{aligned}
> $$

代入 Steffensen 方法的迭代格式可得:

$$
\begin{aligned}
x_{k+1} - x_\star &= \left(x_k - \frac{(f(x_k))^2}{f(x_k+f(x_k)) - f(x_k)}\right) - x_\star \\
&= (x_k - x_\star) - \frac{(f'(x_\star))^2(x_k-x_\star)^2 + f'(x_\star)f''(x_\star)(x_k-x_\star)^3 + O((x_k-x_\star)^4)}{(f'(x_\star))^2(x_k-x_\star) + \frac{1}{2}f''(x_\star)f'(x_\star)(f'(x_\star)+3)(x_k-x_\star)^2 + O((x_k-x_\star)^3)} \\
&= \frac{\frac{1}{2}f''(x_\star)f'(x_\star)(f'(x_\star)+1)(x_k-x_\star)^3 + O((x_k-x_\star)^4)}{(f'(x_\star))^2(x_k-x_\star) + \frac{1}{2}f''(x_\star)f'(x_\star)(f'(x_\star)+3)(x_k-x_\star)^2 + O((x_k-x_\star)^3)} \\
&= \frac{f''(x_\star)}{2f'(x_\star)}(f'(x_\star)+1)(x_k-x_\star)^3 + O((x_k-x_\star)^3)
\end{aligned}
$$

因此当 $f'(x_\star)=-1$ 或 $f''(x_\star)=0$ 时，Steffensen 方法至少局部 3 次收敛.

Problem 3

试给出至少两种数学上不等价的周期函数的插值方法.

Problem 4

试描述 Remez 算法，并证明每步迭代中的类 Vandermonde 系统总具有唯一解.

Problem 5

设 $f(x), f(x \pm h), f(x \pm 2h)$ 已知.
试给出计算 $f''(x)$ 的五点差分格式，并估计最优步长 h.

Problem 6

试推导 Gauss 型求积公式的 Lanczos 算法.

Problem 7

试推导离散 Fourier 逆变换公式.

Problem 8

试使用一次样条基函数的有限元方法将如下初值问题离散化:

$$-u''(x) + \lambda u(x) = v(x)u(x)$$
$$u(0) = 0,\ u(1) = 1$$

请解释所得矩阵中的非零元的计算方法.