Notes on Numerical Analysis

Matthew Mo

2020 年 6 月 30 日

1 Introduction and Math Basics

Reference *Numerical Analysis*

1.1 Rounding/Chopping

- Truncation/Rounding Error
- Roundoff Error

t 位有效数字 ⇒t 是最大非负整数, 使得

$$\frac{|p - p^*|}{|p|} < 5 \times 10^{-t} \tag{1}$$

为了降低这些误差, 可以利用一下变换:

- $\sqrt{x + \varepsilon} - \sqrt{x} = \frac{\varepsilon}{\sqrt{x+\varepsilon}+x}$
- $\ln(x + \varepsilon) - \ln(x) = \ln\left(1 + \frac{\varepsilon}{x}\right)$
- $1 - \cos x = \sin\left(\frac{x}{2}\right)^2$
- $\exp(x) = 1 + \frac{x}{2} + \frac{x^2}{6} + \dots$
- $x^3 + x^2 + 1 \Rightarrow 1 + x^2(x + 1)$

1.2 Algorithm and Convergence

Stability 输入的小改变只导致输出的小改变
Conditional Stability 仅限于某些输入
...

2 Equation Solution

2.1 Bisection

算法: 略

收敛条件:$|\boldsymbol{p}_n - \boldsymbol{p}_{n-1}| \leq \varepsilon$

前向误差: $|x_N - x^*|$

后向误差: $|f(x_N)|$

敏感性:

$$f(x) = 0 \to f(x + \Delta x) + \varepsilon g(x + \Delta x) = 0 \Delta x \approx -\varepsilon \frac{g(x)}{f'(x)}$$

对于 Wilkinson 多项式 $f(x) = \prod_{i=1}^{1} 6(x - i)$,$\Delta x \approx 6.14 \times 10^1 3\varepsilon$

收敛速度: 线性,$|p_n - p| \leq \frac{b-a}{2^n}$, 初始区间为 $[a, b]$

2.2 Fixed Point Iteration

p 是一个不动点, 若 $f(p) = p \Leftrightarrow f(p) - p = 0$.

Theorem (Existence of Fixed Point) If $g : X \to X$ is surjective, then exists $x \in X, s.t. g(x) = x$

Corollary $X = [a, b], g \in C[a, b], |g'(x)| < 1$, then the fixed point is **unique**.

Algorithm

$x_0 =$ given value
$x_n = f(x_{n-1})$
Stop until $\lvert x_n - x_{n-1}\rvert < \varepsilon$

Theorem (Convergence) If g has unique FP on $[a, b]$, then algorithm converges to fixed point p.

Corollary $|x_n - p| \leq k^n max p_0 - a, b - p_0 \wedge |x_n - p| \leq \frac{k^n}{1-k} |x_1 - x_0|$

2.3 Newton Method

考虑二阶泰勒展开

$$f(x) = f(x_0) + f'(x)(x - x_0) + \frac{1}{2} f''(\xi)(x - x_0^2)$$

若 $x - x_0$ 很小, 则

$$0 = f(p) \approx f(x_0) + f'(x_0)(p - x_0) \Rightarrow p \approx x_0 - \frac{f(x_0)}{f'(x_0)}$$

得到迭代步:

$$p_n \approx p_n - 1 - \frac{f(p_{n-1})}{f'(p_{n-1})}$$

Theorem (Convergence) if $f \in C^2[a, b], p \in [a, b] s.t. f(p) = 0, f'(p) \neq 0s$, exists $\delta > 0, s.t. p_n \to p$ for any initial $p_0 \in [p - \delta, p + \delta]$

Note Need to compute derivatives!

2.3.1 Secant Method

$$f'(p_{n-1}) = \lim_{x \to p_{n-1}} \frac{f(x) - f(p_{n-1})}{x - p_{n-1}}$$

使用 p_{n-2} 代替 x, 有割线法迭代 (之后衍生出 BFGS 等一众拟牛顿法):

$$p_n \approx p_n - 1 - \frac{f(p_{n-1})(p_{n-2} - p_{n-1})}{f(p_{n-2}) - f(p_{n-1})}$$

Convergenece

$$e_{i+1} \approx \left| \frac{f''(r)}{2f'(r)} \right| e_i e_{i-1}$$

$\Rightarrow$

$$e_{i+1} \approx \left| \frac{f''(r)}{2f'(r)} \right|^a e_i^a, a = 1 + \varphi = \frac{1 + \sqrt{5}}{2} \approx 1.65$$

Note False Position Method(Regula Falsi) ?

Muller's Method 使用二次函数而非切线:

$$\text{given } x_0, x_1, x_2, \text{find } a, b, c, s.t. P(x) = a(x - x_2)^2 + b(x - x_2) + c$$

迭代公式:

$$x_3 = x_2 - \frac{2c}{b + sgn(b)\sqrt{b^2 - 4ac}}$$

2.3.2 Analysis on Error

Theorem $g \in C[a, b], g(x) \in [a, b], |g'(x)| \leq 1 \Rightarrow p_n = g(p_{n-1})$ 线性收敛到 p.

Theorem p 是 g 的一个不动点,$g'(p) = 0, g''(p)$ 在区间 S 上连续并且有上界 M, 则存在 $\delta > 0, s.t.$ 不动点迭代序列在 $[p - \delta, p + \delta]$ 二次收敛于 p., 且

$$|p_n - p| \leq \frac{M}{2} |p_{n-1} - p|^2$$

2.3.3 Zero Point Multiplicity

Definition 一个 f 的根是 m 重的, 若 $f(x) = (x - p)^m q(x) \wedge \lim_{x \to p} \neq 0$

Theorem iff $f^{(i)}(p) = 0, \forall i = 1...(m - 1), f^{(m)} = 0, p$ 是 m 重根.

Solution $\mu(x) = f(x)/f'(x)$

Failure of NM $f(x) = 4x^4 - 6x^2 - 11/4, x_0 = 1/2$

2.3.4 Other Methods

- IQI Method
- Brent's Method

3 Interpolation and Polynomial Approx.

Weierstrass Approximation Theorem 对于任何 $\varepsilon > 0$, 存在多项式 $p, s.t. |p(x) - f(x)| \leq \varepsilon$

3.1 Lagrange Polynomial

$$p(x) = \sum_{k=0}^{n} f(x_k) L_{n,k}(x)$$

$$\text{where } L_{n,k} = \frac{(x - x_0) \ldots (x - x_{k-1})(x - x_{k+1}) \ldots (x - x_n)}{(x_k - x_0) \ldots x_k - x_{k-1})(x_k - x_{k+1}) ... (x_k - x_n)}$$

Theorem $f \in C^m[a, b], given x_k, f(x_k), \exists\xi, \forall x \in [a, b], f(x) = p(x) + \frac{f^{(n+1)}(xi)}{(n+1)!} \prod_{i=0} n(x - x_i)$

Runge Phenomenon 误差并不一定随多项式阶数提高而降低 $e.g. f(x) = \frac{1}{1+25x^2}$! 它们在边界上有很大的高阶导数 (Cauchy-Lorentz 函数). 高阶拉格朗日多项式 + 均匀采样点会导致龙格现象 $\Rightarrow$ 使用不均匀的 sample, 如 Chebyshev 多项式.

Difficulty 难以决定到底用何阶多项式.

3.1.1 Neville Method

Definition $P_{m_1,\ldots,m_k}$ is Lagrange Polynomialon $x_{m_1}, \ldots, x_{m_k}$

Theorem $P_{1,2,\ldots,k}(x) = \frac{(x - x_j)P_{1,2,\ldots,j-1,j+1,\ldots,k} - (x - x_i)P_{1,2,\ldots,i-1,i+1,\ldots,k}}{x_i - x_j}$

Corollary $P_{1,2,\ldots,k}(x) = \frac{(x - x_1)P_{2,\ldots,k} - (x - x_k)P_{1,\ldots,k-1}}{x_k - x_1}$

可用如下形式计算 P:

P_1			
P_2	P_{12}		
P_3	P_{23}	P_{123}	
P_4	P_{34}	P_{234}	P_{1234}

Neville 法常常用于外插.

3.2 Newton Polynomial

3.2.1 Divided Difference

Definition 均差

$$= f(x_i)$$

$$[x_{j_0}, \ldots, x_{j_k}] = \frac{[x_{j_1}, \ldots, x_{j_k}] - [x_{j_0}, \ldots, x_{j_{k-1}}]}{x_{j_k} - x_{j_0}}$$

若 $j_0, \ldots, j_k$ 是连续的下标.

给出以下均差格式是方便的:

$$
\begin{array}{c|ccccc}
x_0 & [x_0] & & & & \\
 & & [x_0x_1] & & & \\
x_1 & [x_1] & & [x_0x_1x_2] & & \\
 & & [x_1x_2] & & [x_0x_1x_2x_3] & \\
x_2 & [x_2] & & [x_1x_2x_3] & & [x_0x_1x_2x_3x_4] \\
 & & [x_2x_3] & & [x_1x_2x_3x_4] & \\
x_3 & [x_3] & & [x_2x_3x_4] & & \\
 & & [x_3x_4] & & & \\
x_4 & [x_4] & & & &
\end{array}
$$

可以给出 Newton 内插公式

$$P_n(x) = \sum_i c_i N_i . c_i = [x_0, ..., x_n], N_0(x) = 1, N_i(x) = \prod_j^{i-1} (x - x_j)$$

对于相等间隔的采样点 $x_j = x_0 + jh$, 有

$$[x_i x_{i+1} \dots x_{i+k}] = \frac{1}{k! h^k} \Delta^k y_i$$

以及前向差分 (Forward Difference)

$$\Delta^0 y_i = y_i, \Delta^k y_i = \Delta^{k-1} y_{i+1} - \Delta^{k-1} y_i$$

得到牛顿-格里高利 I 型插值公式

$$P_n(x) = y_0 + \sum_{i=0}^{n} \binom{t}{h} \Delta^u y_0, x = x_0 + th$$

也可采用后向差分 (Backward Difference)

$$\nabla^0 y_{n-j} = y_{n-j}, \nabla^k y_{n-j} = \nabla^{k-1} y_{n-j} - \nabla^{k-1} y_{n-j-1}$$

以及 Newton-Gregory II 插值公式

$$I_n(x) = y_n + \sum_{i=1}^{n} \binom{s}{i} \nabla^i y_n, x = x_n + sh.$$

有牛顿均差公式

$$[x_0 x_1 \dots x_k] = \frac{\Delta^k y_k}{k! h^k}$$

3.3 Hermite Interpolation

Target 内插函数值和导数值!

以下的 2n+1 阶函数内插了两者

$$H_{2n+1}(x) = \sum_{j=0}^{n} f(x_j) H_{n,j}(x) + \sum_{j=0}^{n} f'(x_j) \widehat{H}_{n,j}(x)$$

其中

$$
\begin{aligned}
H_{n,j}(x) &= (1 - 2(x - x_j)L'_{n,j}(x_j)))L^2_{n,j}(x) \\
\widehat{H}_{n,j}(x) &= (x - x_j)L^2_{n,j}(x)
\end{aligned}
$$

误差

$$\prod_{i=0}^{n}(x - x_j)\frac{f^{(2n+2)}(\xi)}{(2n+2)!}$$

写成牛顿迭代的形式, 以迭代计算

$$
\begin{aligned}
&H_{2n+1}(x) = [z_0] + \sum_{k=1}^{2n+1}[z_0 \dots z_k](x - z_0)(x - z_1)\dots(x - z_{k-1}) \\
&\text{where } z_{2i} = z_{2i+1} = x_i, [z_{2i}, z_{2i+1}] = f'(z_{2i}) = f'(x_i)
\end{aligned}
$$

Theorem $x_i \in [a, b], f \in C^n[a, b], \exists\xi \in [a, b], [x_0 \dots x_k] = \frac{f^{(n)}(\xi)}{n!}$

3.4 Cubic Spline Interpolation

一种分段连续的逼近

Definition 一个对函数 f 的三次样条内插函数 S, 且插值点 $a = x_0 < x_1 < \cdots < x_n = b$ 需要满足:

1. $S(x)$ 是分段三次的, 由在 $[x_j, x_j + 1]$ 上定义的函数 $s_j(x)$ 组成
2. $S(x_j) = f(x_j)$
3. $s_{j+1}(x_{j+1}) = s_j(x_{j+1})$ 函数值连续性
4. $s'_{j+1}(x_{j+1}) = s'_j(x_{j+1})$ 导数连续性
5. $s''_{j+1}(x_{j+1}) = s''_j(x_{j+1})$ 二阶导数连续性
6. 满足下列之一的边界条件:
   - $S''(x_0) = S''(x_n) = 0$ Natural
   - $S'(x_0) = f'(x_0), S'(x_n) = f'(x_n)$ Clamped

这些三次函数的形式

$$s_j(x) = a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3 s'_j(x) = b_j + 2c_j(x - x_j) + 3d_j(x - x_j)^2 s''_j(x) = 2c_j + 6d_j(x - x$$

对于自然边界条件

$$A = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ h_0 & 2(h_0+h_1) & h_1 & \dots & \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & \cdots & h_{n-2} & 2(h_{n-1}+h_{n-2}) & h_{n-1} \\ 0 & \cdots & 0 & 0 & 1 \end{pmatrix}, \text{which is diagonally dominant}$$

$$b = \begin{pmatrix} 0 \\ 3/h_1(a_2-a_1) - 3/h_0(a_1-a_0) \\ \vdots \\ 3/h_{n-1}(a_n-a_{n-1}) - 3/h_{n-2}(a_{n-1}-a_{n-2}) \\ 0 \end{pmatrix}, x = (c_0, \dots, c_n)^T, AX = b$$

对于 clamped 边界条件

$$A = \begin{pmatrix} 2h_0 & h_0 & 0 & \dots & 0 \\ h_0 & 2(h_0+h_1) & h_1 & \dots & \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & \cdots & h_{n-2} & 2(h_{n-1}+h_{n-2}) & h_{n-1} \\ 0 & \cdots & 0 & h_{n-1} & 2h_{n-1} \end{pmatrix}, \text{which is diagonally dominant}$$

$$b = \begin{pmatrix} 3/h_1(a_2-a_1) - 3/f'(a) \\ 3/h_1(a_2-a_1) - 3/h_0(a_1-a_0) \\ \vdots \\ 3/h_{n-1}(a_n-a_{n-1}) - 3/h_{n-2}(a_{n-1}-a_{n-2}) \\ 3f'(b) - 3/h_{n-1}(a_n-a_{n-1}) \end{pmatrix}, x = (c_0, \dots, c_n)^T, AX = b$$

3.5 Bernstein Polynomials

B-样条函数, 用于在参数曲线上拟合

$$B_i^n(t) = \binom{n}{i}(1-t)^{n-i}t^i$$

以及

$$\boldsymbol{x}(t) = \sum_i B_i^3(t)\boldsymbol{p}(t)$$

4 Numerical Differentiation and Integration

5 Linear/Polynomial System Approx.

5.1 Normal Equation (on LP/Linear Programming)

$$\boldsymbol{Ax} = \boldsymbol{b} \Rightarrow \overline{\boldsymbol{x}} = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T\boldsymbol{b}$$

5.2 Discrete Least Mean Square

使用 L2-范数衡量误差:

$$E = ||\boldsymbol{y} - f(\boldsymbol{x}; \boldsymbol{\theta})||_2^2$$

5.3 As a Hilbert Space

给出函数空间上的内积, 如果能找到一组正交基 ϕ_i, 则有 Gram 矩阵

$$\boldsymbol{G} = (g_{ij}) = (\langle \phi_i, \phi_j \rangle)$$

将函数表示为 $p(x) = \sum_k c_k \phi_k(x)$ 则可表示内积为

$$\langle f, \phi_j \rangle = \sum_k c_k g_{jk} \Rightarrow \boldsymbol{Gc} = \langle f, \boldsymbol{\phi} \rangle$$

考虑普通的多项式逼近 $f(x) : P_n(x) = \sum_k a_k x^k$ 的误差

$$E[f] = \int_{[a,b]} (f(x) - P_n(x))^2 dx$$

为了计算系数 a_j, 我们要解方程

$$\sum_{k=0}^{n} a_k \int_{[a,b]} x^{j+k} dx = \int_{[a,b]} x^f f(x) dx$$

这个方程当采样点数增加, 条件数趋向于无穷 $\Rightarrow$ 数值计算的困难性.

Theorem ϕ_j 是线性无关的, 如果它们的阶不同.

我们可以考虑广义的带权内积

$$\langle f, g \rangle = \int_X f(x)g(x)w(x)dx, w(x)|_{x\in X} > 0$$

给出内积之后, 就可以通过 Gram-Schimdt 正交化得出一组正交基, 当 $w(x) \equiv 1$ 对应的正交基是 Legendre 多项式.

Theorem $\langle Q, \phi_n \rangle$ 若 Q 的阶数小于 ϕ_n

5.4 Chebyshev Polynomials

$X = [-1,1], w(x) = \frac{1}{\sqrt{1-x^2}}$ 给出切比雪夫多项式

$$T_n(x) = \cos(n \arccos(x)),$$
$$T_0(x) = 1, T_1(x) = x,$$
$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$$

它们有单根 $x_k = \cos\left(\frac{2k-1}{n}\frac{\pi}{2}\right)$ 那么系数

$$c_k = \frac{2}{\pi}\int_0^{\pi} f(cos(\phi))k\phi d\phi$$

以及 $\langle T_i, T_j\rangle = \frac{\pi}{2}\delta_{ij}, i+j \neq 0 \wedge \langle T_0, T_0\rangle = \pi$

Theorem 切比雪夫多项式有零点 $x_k = \cos\left(\frac{2k-1}{n}\frac{\pi}{2}\right)$ 和极值 $x_k' = \cos\left(\frac{k\pi}{n}\right)$

5.4.1 Monic CP

首一 CP:

$$\widetilde{T}_n(x) = \frac{1}{2^{n-1}}T_n(x)$$

那么

$$\widetilde{T}_n(x) = x\widetilde{T}_{n-1}(x) - \frac{1}{4}\widetilde{T}_{n-2}(x)$$

有零点 $x_k = \cos\left(\frac{2k-1}{n}\frac{\pi}{2}\right)$ 和极值 $x_k' = \cos\left(\frac{k\pi}{n}\right)$. 设 $\widetilde{\Pi}_n$ 是所有 n 阶及以下首一多项式, 有

Theorem $\forall P_n(x) \in \widetilde{\Pi}_n, x \in [-1,1], \frac{1}{2^{n-1}} = \max\ |\widetilde{T}_n(x)| \leq \max\ |P_n(x)|$

Corollary

6 Iterative Techs in Matrix Algebra

7 ODEs

8 Nonlinear Systems

9 Eigenvalues

10 PDEs