1 插值

1.1 Hermite插值

•**Hermite插值**

$$h_i = \left(1 - 2(x - x_i)\sum_{j\neq i}\frac{1}{x_i - x_j}\right) l_i^2(x)$$

$$g_i = (x - x_i) l_i^2(x)$$

1.2 三次样条M关系式

•$S(x)$

$$S(x) = \frac{(x_{i+1}-x)^3 M_i + (x-x_i)^3 M_{i+1}}{6h_i} + \frac{(x_{i+1}-x)y_i + (x-x_i)y_{i+1}}{h_i}$$
$$-\frac{h_i}{6}[(x_{i+1}-x)M_i + (x-x_i)M_{i+1}],\ x\in[x_i, x_{i+1}]$$

•M_i的递推式

$$\begin{cases} \mu_i M_{i-1} + 2M_i + \lambda_i M_{i+1} = d_i,\ i = 1,2,\cdots,n-1 \\ \lambda_i = \frac{h_i}{h_i + h_{i-1}},\ \mu_i = 1 - \lambda_i \\ d_i = 6f[x_{i-1}, x_i, x_{i+1}] \end{cases}$$

•边界条件为:$M_0 = M_n = 0$

$$\begin{bmatrix} 2 & \lambda_1 & & & \\ \mu_2 & 2 & \lambda_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \mu_{n-2} & 2 & \lambda_{n-2} \\ & & & \mu_{n-1} & 2 \end{bmatrix} \begin{bmatrix} M_1 \\ M_2 \\ \vdots \\ M_{n-2} \\ M_{n-1} \end{bmatrix} = \begin{bmatrix} d_1 - \mu_1 M_0 \\ d_2 \\ \vdots \\ d_{n-2} \\ d_{n-1} - \lambda_{n-1} M_n \end{bmatrix}$$

•边界条件为:$S'(x_0) = m_0, S'(x_n) = m_n$

$$\begin{cases} 2M_0 + M_1 = \frac{6}{h_0}[f[x_0, x_1] - m_0] = d_0 = f[x_0, x_0, x_1] \\ M_{n-1} + 2M_n = \frac{6}{h_{n-1}}[m_n f[x_{n-1}, x_n]] = d_n = f[x_{n-1}, x_n, x_n] \end{cases}$$

$$
\begin{bmatrix}
2 & 1 & & & & \\
\mu_1 & 2 & \lambda_1 & & & \\
 & \mu_2 & 2 & \lambda_2 & & \\
 & & \ddots & \ddots & \ddots & \\
 & & & \mu_{n-2} & 2 & \lambda_{n-1} \\
 & & & & 1 & 2
\end{bmatrix}
\begin{bmatrix} M_0 \\ M_1 \\ M_2 \\ \vdots \\ M_{n-2} \\ M_{n-1} \end{bmatrix}
=
\begin{bmatrix} d_0 \\ d_1 \\ d_2 \\ \vdots \\ d_{n-1} \\ d_n \end{bmatrix}
$$

•**边值条件为被插函数以$x_n - x_0$为基本周期**　即$m_0 = m_n$，$M_0 = M_n$，将$S'(x_0) = S'(x_n)$加入方程组，化为n变量，n个方程组。

1.3 三次样条m关系式

•**S(x)**

$$
\begin{aligned}
S(x) = &(1 - 2\frac{x - x_i}{x_i - x_{i+1}})(\frac{x - x_{i+1}}{x_i - x_{i+1}})^2 y_i + (x - x_i)(\frac{x - x_{i+1}}{x_i - x_{i+1}})^2 m_i \\
&+ (1 - 2\frac{x - x_{i+1}}{x_{i+1} - x_i})(\frac{x - x_i}{x_{i+1} - x_i})^2 y_{i+1} + (x - x_{i+1})(\frac{x - x_i}{x_{i+1} - x_i})^2 m_{i+1}
\end{aligned}
$$

•**递推式**

$$
\begin{cases}
\lambda_i m_{i-1} + 2m_i + \mu_i m_{i+1} = c_i, \ i = 1, 2, \cdots, n-1 \\
\lambda_i = \frac{h_i}{h_i + h_{i-1}}, \ \mu_i = 1 - \lambda_i \\
c_i = 3[\lambda_i y[x_{i-1}, x_i] + \mu_i y[x_i, x_{i+1}]]
\end{cases}
$$

2 拟合

•**矛盾方程组**　$AX = Y$无解。而$A^T AX = A^T Y$为的解为最小二乘解(使$||AX - Y||_2$最小)。

3 非线性方程求解

•**对分法(二分法)**

•**不动点迭代的收敛**

$$\begin{cases} x\in[a,b]\Rightarrow a\le\varphi(x)\le b \\ \varphi(x)\in C^1[a,b]\wedge(\exists 0<L<1, s.t., \forall x\in[a,b], |\phi'(x)|\le L) \end{cases}$$

$\Rightarrow$

$$\begin{cases} \text{在}[a,b]\text{上有唯一不动点}x^*\text{，而且迭代格式对任意初值均收敛于}x^* \\ |x^*-x_k|\le\frac{L^k}{1-L}|x_1-x_0| \end{cases}$$

•**迭代格式收敛阶**　若存在$M>0$, $\lim\limits_{k\to\infty}\frac{|e_{k+1}|}{|e_k|^n}=\lim\limits_{k\to\infty}\frac{|x_{k+1}-\alpha|}{|x_k-\alpha|^n}=M$，则称迭代格式收敛阶为n.

•**误差阶计算的一个方法**　若$\begin{cases} \varphi^{(k)}(x^*)=0,\ k=0,1,\cdots,p-1 \\ \varphi^p(x^*)\ne 0 \end{cases}$, 则展开后有$\lim\limits_{k\to\infty}\frac{x_{k+1}-x^*}{(x_k-x^*)^p}=M$,故p阶收敛.

•**弦截法的误差阶**　先写成

$$e_{k+1}=\frac{x_k-x_{k-1}}{f(x_k)-f(x_{k-1})}\cdot\frac{f(x_k)/e_k-f(x_{k-1})/e_{k-1}}{x_k-x_{k-1}}\cdot e_ke_{k-1}\ ,$$

再对$f(x_k)=f(x^*+e_k)$泰勒展开,且令$|e_{k+1}|\sim A|e_k|^\alpha$,代入化简,得$\alpha=\frac{1+\alpha}{\alpha}$.

4　求解线性方程组的直接法

•**Doolittle**　$A=LU$,L是单位下三角,U是上三角,先求U行,再求L列(先求非单位三角阵).

•**Crout**　$A=LU$,L是下三角,U是单位上三角,先求L列,再求U行(先求非单位三角阵).

•**追赶法**　三对角方程组

•LDL^T**分解**　对称正定矩阵，L是单位下三角矩阵，D是对角矩阵.

5　求解线性方程组的迭代方法

•**行对角占优,列对角占优,对角占优**　大于行(列)内其他元素和即为行(列)占优. 统称对角占优.

5.1 Jacobi迭代

•**Jacobi迭代** $D = diag\{a_{11}, \ldots, a_{nn}\}$,则有

$$X^{(k+1)} = D^{-1}(D-A)X^{(k)} + D^{-1}b$$

•**若M严格对角优，则可逆**

•**当A严格对角优，Jacobi迭代收敛**

5.2 Gauss-Seidel迭代

•**Gauss-Seidel迭代** 令$A = L + D + U$,则

$$(L+D)X^{(k+1)} + UX^{(k)} = b$$

从而,

$$X^{(k+1)} = -(D+L)^{-1}UX^{(k)} + (D+L)^{-1}b$$

•**当A严格对角优，Gauss-Seidel迭代收敛**

•**当A正定对称时，Gauss-Seidel迭代收敛**

5.3 松弛迭代——SOR迭代

•**SOR迭代** 对结果加权ω,剩余权重$(1-\omega)$给$X^{(k)}$

•**SOR迭代收敛必要条件** $0 < \omega < 2$

•**若A对称正定，则在上述条件下恒收敛**

6 数值积分和数值微分

$I(f)$表示函数$f(x)$精确积分值,$I_n(f)$表示近似积分值.

$I(f) = \int_a^b f(x)dx,\ I_n(f) = \sum\limits_{i=0}^{n} \alpha_i f(x_i)$

构造数值积分就是要确定α_i的值

•**代数精度** 若$I_n(f)$满足

$$E_n(x^k) = I(x^k) - I_n(x^k) = 0,\ k = 0, 1, \ldots, m$$
$$E_n(x^{m+1}) \neq 0$$

则称$I_n(f)$具有m阶代数精度.此时对任意不高于m次的多项式$f(x)$都有$I(f) = I_n(f)$.

要确定一个数值积分的代数精度，可以从$x, x^2, \ldots$开始代,直到不为0.

6.1 插值型数值积分

•插值型数值积分代数精度 n阶插值多项式形式的数值积分公式至少有n阶代数精度

6.2 牛顿-柯特斯积分

•梯形积分 $T(f)=\frac{b-a}{2}[f(a)+f(b)]$

•梯形积分代数精度和误差 一阶代数精度.误差为:

$$E_1(x)=\int_a^b \frac{f''(\xi)}{2!}(x-a)(x-b)dx=-\frac{f''(\eta)}{12}(b-a)^3$$

•Simpson $S(f)=\frac{b-a}{6}\left[f(a)+4f(\frac{a+b}{2})+f(b)\right]$

•Simpson积分代数精度和误差 三阶代数精度.误差为:

$$E_2(x)=\int_a^b \frac{f^{(4)}(\xi)}{4!}x(x-a)(x-\frac{a+b}{2})(x-b)dx=-\frac{f^4(\eta)}{2880}(b-a)^5$$

•Newton-Cotes积分误差

$$\begin{cases} \text{若}m\text{为奇数,则}E_n(f)=\frac{f^{(n+1)}(\eta)}{(n+1)!}\int_a^b(x-x_0)(x-x_1)\dots(x-x_n)dx \\ \text{若}m\text{为偶数,则}E_n(f)=\frac{f^{(n+2)}(\eta)}{(n+2)!}\int_a^b x(x-x_0)(x-x_1)\dots(x-x_n)dx \end{cases}$$

6.3 复化数值积分

•复化梯形积分计算公式

$$T(h)=T_n(f)=h\left[\frac{1}{2}f(a)+\sum_{i=0}^{n-1}f(a+ih)+\frac{1}{2}f(b)\right],\ h=\frac{b-a}{n}$$

•复化梯形积分公式截断误差

$$E_n(f)=-n\frac{h^3}{12}f''(\xi)=-\frac{(b-a)^3)}{12n^2}f''(\xi)$$

•复化Simpson积分

$$S_n(f)=\frac{h}{3}\left[f(a)+4\sum_{i=0}^{m-1}f(x_{2i+1})+2\sum_{i=1}^{m-1}f(x_{2i})+f(b)\right],\ h=\frac{b-a}{n},\ n=2m$$

•复化Simpson积分公式截断误差

$$E_n(f)=-m\frac{(2h)^5}{2880}f^{(4)}(\xi)=-\frac{(b-a)^5}{2880m^4}f^{(4)}(\xi)$$

6.4 自动控制误差的复化积分

•梯形积分误差控制

$$
\begin{aligned}
let\ H_n(f) &= h_n \sum_{i=0}^{n-1} f(x_{i+1/2}),\ h_{2n} = \frac{b-a}{2n} \\
T_{2n} &= \frac{1}{2}[T_n(f) + h_n(f)] \\
&= \frac{T_n}{2} + h_{2n} \sum_{i=1}^{n} f(a + (2i-1)h_{2n})
\end{aligned}
$$

•梯形积分后验误差　由$I(f) - T_n(f) \approx 4(I(f) - T_{2n}(f))$得:

$$
I(f) - T_{2n}(f) \approx \frac{1}{3}(T_{2n}(f) - T_n(f))
$$

•**Simpson积分误差控制**

$$
S_{2n}(f) = \frac{S_n(f)}{2} + \frac{1}{6}(4H_{2n}(f) - H_n(f))
$$

6.5 Romberg积分

•**Romberg积分**

$$
\begin{aligned}
&I(f) \approx T_{2n}(f) + \tfrac{1}{3}(T_{2n}(f) - T_n(f)) = S_n(f) \\
&I(f) \approx S_{2n}(f) + \tfrac{1}{15}(S_{2n}(f) - S_n(f)) = C_n(f) \\
&\ldots \\
&R_{k,j} = R_{k,j-1} + \tfrac{R_{k,k-1} - R_{k-1,j-1}}{4^{j-1}-1}
\end{aligned}
$$

6.6 高斯积分

•积分公式代数精度最高为$2n-1$

•**Legendre多项式**　$L_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n$

•高斯积分　对$I(f) = \int_{-1}^{1} f(x)dx$,选取Legendre多项式$L_n(x)$的$n$个零点为数值积分节点,则有

$$
I_n(f) = \sum_{i=1}^{n} \alpha_i^{(n)} f(x_i^{(n)}).
$$

它具有$2n-1$阶代数精度

6.7 数值微分

•**向前差商**

$$f'(x_0) \approx \frac{f(x_0+h)-f(x_0)}{h}$$
$$R(x) = -\frac{h}{2}f''(\xi) = O(h)$$

•**向后差商**

$$f'(x_0) \approx \frac{f(x_0)-f(x_0-h)}{h}$$
$$R(x) = \frac{h}{2}f''(\xi) = O(h)$$

•**中心差商**

$$f'(x_0) \approx \frac{f(x_0+h)-f(x_0-h)}{2h}$$
$$R(x) = \frac{h^2}{6}f''(\xi) = O(h^2)$$

•**步长选取** 中心差商为例,舍入误差用$\frac{e}{h}$估计,有

$$\text{总误差为}\frac{h^2}{6}M_3 + \frac{e}{h}$$

求导可知,达最小值时,$h = \sqrt[3]{\frac{3e}{M_3}}$

•**事后估计** $\left[D(h,x) - D(\frac{h}{2},x)\right] < \epsilon$时,步长$h$就是合适的步长

•**插值型微分误差**

$$R(x) = \frac{d}{dx}\left(\frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{\substack{i=0\\i\neq j}}^{n}(x_j - x_i)\frac{f^{(n+1)}(\xi)}{(n+1)!}\right)$$

7 常微分方程数值解

7.1 Runge-Kutta方法

•**2阶Runge-Kutta**

$$\begin{cases} c_1 + c_2 = 1 \\ 2c_2a = 1 \\ 2c_2b = 1 \\ y_{n+1} = y_n + h(c_1k_1 + c_2k_2) \\ k_1 = f(x_n, y_n) \\ k_2 = f(x_n + ah, y_n + bhk_1) \end{cases}$$

7.2 线性多步法

•线性多步法

$$\begin{cases} f(x_{n+1}) = f(x_{n-p}) + \int_{x_{n-p}}^{x_{n+1}} f(x,y)dx \\ \text{显示格式积分节点为}\{x_n, x_{n-1}, \dots, x_{n-q}\} \\ \text{隐式格式积分节点为}\{x_{n+1}, x_n, \dots, x_{n+1-q}\} \end{cases}$$

8 计算矩阵的特征值和特征向量

8.1 幂法

•幂法　有$X^{(k)} = \alpha_1\lambda_1^k v_1 + \cdots + \alpha_n\lambda_n^k v_n$

$$\begin{cases} \text{按模最大特征值只有一个:} \begin{cases} \lambda_1 \approx x_i^{(k+1)}/x_i^{(k)} \\ v_1 = X^{(k)} \end{cases} \\ \text{按模最大特征值为两相反数:} \begin{cases} \lambda_1 \approx \sqrt{x_i^{(k+2)}/x_i^{(k)}} \\ v_1 = X^{(k+1)} + \lambda_1 X^{(k)} \\ v_2 = X^{(k+1)} - \lambda_1 X^{(k)} \end{cases} \end{cases}$$

•规范化

$$\begin{cases} Y^{(k)} = X^{(k)}/||X^{(k)}||_\infty \\ X^{(k+1)} = AX^{(k)} \\ \text{收敛于一个向量:} \begin{cases} \lambda_1 \approx \max\limits_{1\le i\le n} |x_i^{(k+1)}| \\ v_1 = Y^{(k)} \end{cases} \\ \text{偶数列和奇数列收敛于反号向量:} \begin{cases} \lambda_1 \approx -\max\limits_{1\le i\le n} |x_i^{(k+1)}| \\ v_1 = Y^{(k)} \end{cases} \\ \text{偶数列和奇数列收敛于两个不同向量:} \begin{cases} \lambda_1 \approx \sqrt{x_i^{(k+1)}/y_i^{(k-1)}} \\ \lambda_2 = -\lambda_1 \\ v_1 = X^{(k+1)} + \lambda_1 X^{(k)} \\ v_2 = X^{(k+1)} - \lambda_1 X^{(k)} \end{cases} \end{cases}$$

•反幂法取A^{-1}即可

8.2 实对称矩阵的Jacobi方法

•Givens变换结果 若$Q = Q(p, q, \theta)$,则有:

$$\begin{cases} b_{ip} = b_{pi} = a_{pi} cos\theta - a_{qi} sin\theta, \ i \neq p, q \\ b_{iq} = b_{qi} = a_{pi} sin\theta + a_{qi} cos\theta, \ i \neq p, q \\ b_{pp} = a_{pp} cos^2\theta + a_{qq} sin^2\theta - a_{pq} sin2\theta \\ b_{qq} = a_{pp} sin^2\theta + a_{qq} cos^2\theta + a_{pq} sin2\theta \\ b_{pq} = b_{qp} = a_{pq} cos2\theta + \frac{a_{pp} - a_{qq}}{2} sin2\theta \end{cases}$$

为使$b_{pq} = b_{qp} = 0$,令$s = \frac{a_{qq} - a_{pp}}{2a_{pq}}$, $t^2 + 2st - 1 = 0$的绝对值最小根作为$tan\theta$.

$$\begin{cases} b_{ip} = b_{pi} = ca_{pi} - da_{qi}, \ i \neq p, q \\ b_{iq} = b_{qi} = da_{pi} + ca_{qi}, \ i \neq p, q \\ b_{pp} = a_{pp} - ta_{pq} \\ b_{qq} = a_{pp} + ta_{pq} \\ b_{pq} = b_{qp} = 0 \\ b_{ij} = a_{ij}, \ i \neq p, q; \ j \neq p, q \end{cases}$$