01 数值计算的误差

截断误差（方法误差）：当数学模型不能得到精确解时，通常要用数值方法求它的近似解，其近似解与精确解之间的误差称为截断误差。

舍入误差：计算机只能处理有限数位的小数运算，原始数据或中间结果都必须进行四舍五入运算，即原始数据和计算过程可能产生新的误差。

Taylor 公式：$R_n(x)=\frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)^{n+1}$，$\xi\in[x_0,x]$

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

$\frac{f^{(n)}(x_0)}{n!}(x-x_0)^n+R_n(x) \ =\sum_{k=0}^{n}\frac{f^{(k)}(x_0)}{k!}(x-x_0)^k+R_n(x)$

设 x 为准确值，x* 为 x 的一个近似值，称 e = x − x*
为近似值 x 的**绝对误差**，简称**误差**，记为 e。
我们把近似值的误差 e* 与准确值 x 的比值

$$\frac{e^*}{x^*}=\frac{x^*-x}{x^*}$$

称为近似值 x* 的**相对误差**，记作 e_r^*

有效数字：如果近似值 x*的误差限是某一位的半个单位，该位到 x*的第一个非零数字共有 n 位，就说 x*有 n 位**有效数字。** $x^*=\pm10^m\times(a_1+a_2\times10^{-1}+\cdots+a_n\times10^{-(n-1)})$

$|x-x^*|\leqslant\frac{1}{2}\times10^{m-n+1}$

病态问题与条件数：计算函数值 f(x) 时，若 x 有扰动 $\Delta x=x-x^*$，其相对误差为 $\frac{\Delta x}{x}$，函数值 $f(x^*)$ 的相对误差为 $\frac{f(x)-f(x^*)}{f(x)}$，利用 $f(x^*)\approx f(x)+f'(x)(x^*-x)$，相对误差比值 $\left|\frac{f(x)-f(x^*)}{f(x)}\right|/\left|\frac{\Delta x}{x}\right|\approx\left|\frac{xf'(x)}{f(x)}\right|=C_p$ 称为计算函数值问题的**条件数**。一般 $C_p\ge10$ 就认为是病态的。

避免误差危害：避免除数绝对值远远小于被除数绝对值的除法；要避免两相近数相减；要防止“大数”吃掉小数；注意简化计算步骤，减少运算次数和舍入误差。

霍纳算法：$\begin{cases}S_n=a_n\\ S_k=xS_{k+1}+a_k\ (k=n-1,\cdots,2,1,0)\\ P_n(x)=S_0\end{cases}$

$P_n(x)=((a_nx+a_{n-1})x+a_{n-2})x\cdots+a_1)x+a_0$ n 次乘和加

$$P_n(x)=\sum_{i=0}^{n}a_ix^i, b_n=a_n, b_k=a_k+cb_{k+1}, b_0=P(c)$$

Input	a_n	a_{n-1}	a_{n-2}	$\cdots$	a_k	$\cdots$	a_2	a_1	a_0
c		xb_n	xb_{n-1}	$\cdots$	xb_{k+1}	$\cdots$	xb_3	xb_2	xb_1
	b_n	b_{n-1}	b_{n-2}	$\cdots$	b_k	$\cdots$	b_2	b_1	$b_0=P(c)$ Output

Big O(h)：$f(h)=p(h)+O(h^n)$，$g(h)=q(h)+O(h^m)$

$r=min\{m,n\}$ $f(h)+g(h)=p(h)+q(h)+\boldsymbol{O}(h^r)$

$f(h)g(h)=p(h)q(h)+\boldsymbol{O}(h^r)$ $\frac{f(h)}{g(h)}=\frac{p(h)}{q(h)}+O(h^r)$

02 插值法

拉格朗日插值：$L_n(x)=\sum_{i=0}^{n}\left(y_i\frac{\prod_{j=0,j\neq i}^{n}(x-x_j)}{\prod_{j=0,j\neq i}^{n}(x_i-x_j)}\right)=$

$\sum_{i=0}^{n}(y_il_i(x))$ *其中* $l_i(x)=\frac{\prod_{j=0,j\neq i}^{n}(x-x_j)}{\prod_{j=0,j\neq i}^{n}(x_i-x_j)}$

截断误差：$R_n(x)=f(x)-L_n(x)=\frac{f^{(n+1)}(\xi)}{(n+1)!}\omega_{n+1}(x)$

$\omega_{n+1}(x)=(x-x_0)(x-x_1)\cdots(x-x_k)\cdots(x-x_n)$

$\sum_{i=0}^{n}x_i^kl_i(x)=x^k$ $k=0,1,\cdots n$ n 次插值要 **n+1** 个点

牛顿插值：$P_n(x)=a_0+\sum_{i=0}^{n-1}\left(a_{i+1}\prod_{j=0}^{i}(x-x_j)\right)$

$f[x_k,x_{k-1},\dots,x_j]\ =\frac{f[x_k,x_{k-1},\dots,x_{j+1}]-f[x_{k-1},x_{k-2},\dots,x_j]}{x_k-x_j}$

k 阶：$f[x_0,x_1,\cdots,x_k]=\frac{f[x_0,\cdots,x_{k-2},x_k]-f[x_0,x_1\cdots,x_{k-2},x_{k-1}]}{x_k-x_{k-1}}$

$P_n(x)=f(x_0)+f[x_0,x_1](x-x_0)+f[x_0,x_1,x_2](x-x_0)(x-x_1)+\cdots+f[x_0,x_1,\cdots,x_n](x-x_0)\cdots(x-x_{n-1})$

截断误差：$R_n(x)=f[x,x_0,\cdots,x_n](x-x_0)\cdots(x-x_n)$，4 次多项式需要 4 阶均差

x_k	$f(x_k)$	一阶均差	二阶均差
x_0	$f(x_0)$		
x_1	$f(x_1)$	$f[x_0,x_1]$	
x_2	$f(x_2)$	$f[x_1,x_2]$	$f[x_0,x_1,x_2]$

埃尔米特插值：**三点三次**：$P(x_i)=f(x_i)$ $(i=0,1,2)$ 且 $P'(x_1)=f'(x_1)$，$P(x)=f(x_0)+f[x_0,x_1](x-x_0)+f[x_0,x_1,x_2](x-x_0)(x-x_1)+A(x-x_0)(x-x_1)(x-x_2)$ 用**重节点的均差表**；**待定系数法**

其中 A 为待定常数，可由条件 $P'(x_1)=f'(x_1)$ 确定

$$A=\frac{f'(x_1)-f[x_0,x_1]-(x_1-x_0)f[x_0,x_1,x_2]}{(x_1-x_0)(x_1-x_2)}$$

$$R(x)\ =\frac{1}{4!}f^{(4)}(\xi)(x-x_0)(x-x_1)^2(x-x_2)$$

$N_2(x)=f(0)+f[0,1](x-0)+f[0,1,2](x-0)(x-1)$

$H_3(x)=N_2(x)+k(x-0)(x-1)(x-2)$

$H_3'(1)=f'(1)=3$，$4-k=3, k=1$

两点三次：$\begin{matrix}H_3(x_k)=y_k, H_3(x_{k+1})=y_{k+1},\\ H_3'(x_k)=m_k, H_3'(x_{k+1})=m_{k+1}\end{matrix}$

$H_3(x)=\alpha_k(x)y_k+\alpha_{k+1}(x)y_{k+1}+\beta_k(x)m_k+\beta_{k+1}(x)m_{k+1}$

$\alpha_k(x)=\left(1+2\frac{x-x_k}{x_{k+1}-x_k}\right)\left(\frac{x-x_{k+1}}{x_k-x_{k+1}}\right)^2$ $\alpha_{k+1}(x)=(1+$

$2\frac{x-x_{k+1}}{x_k-x_{k+1}}\Big)\left(\frac{x-x_k}{x_{k+1}-x_k}\right)^2 \quad \beta_k(x)=(x-x_k)\left(\frac{x-x_{k+1}}{x_k-x_{k+1}}\right)^2$

$\beta_{k+1}(x)=(x-x_{k+1})\left(\frac{x-x_k}{x_{k+1}-x_k}\right)^2$

$R_3(x)=\frac{1}{4!}f^{(4)}(\xi)(x-x_k)^2(x-x_{k+1})^2,\ \xi\in(x_k,x_{k+1})$

分段线性插值：每个小区间 $[x_k,x_{k+1}]$ 可表示为：

$I_h(x)=\frac{x-x_{k+1}}{x_k-x_{k+1}}f_k+\frac{x-x_k}{x_{k+1}-x_k}f_{k+1}, x_k\leqslant x\leqslant x_{k+1}, k=$

$0,1,\cdots,n-1$ 其中 $I_h(x)\in C[a,b]$，$I_h(x)=f_k$

$\max_{a\leqslant x\leqslant b}|f(x)-I_h(x)|\leqslant\frac{M_2}{8}h^2=O(h^2)$ M 二阶导最大

分段三次埃尔米特插值：

$I_h(x_k)=f_k, I_h'(x_k)=m_k\ I_h(\mathrm{x})\ \ x\in[x_k,x_{k+1}]$

$I_h(x)=\left(1+2\frac{x-x_k}{x_{k+1}-x_k}\right)\left(\frac{x-x_{k+1}}{x_k-x_{k+1}}\right)^2f_k+\left(1+2\frac{x-x_{k+1}}{x_k-x_{k+1}}\right)\left(\frac{x-x_k}{x_{k+1}-x_k}\right)^2f_{k+1}$

$+(x-x_k)\left(\frac{x-x_{k+1}}{x_k-x_{k+1}}\right)^2m_k+(x-x_{k+1})\left(\frac{x-x_k}{x_{k+1}-x_k}\right)^2m_{k+1}$

$\max_{a\leqslant x\leqslant b}|f(x)-I_h(x)|\leqslant\frac{M_4}{384}h^4=O(h^4)$ M 四阶导最大值

三次样条插值：$h_0=x_1-x_0$，$h_{n-1}=x_n-x_{n-1}$

$$S(x)=M_j\frac{(x_{j+1}-x)^3}{6h_j}+M_{j+1}\frac{(x-x_j)^3}{6h_j}+\left(y_j-\frac{M_jh_j^2}{6}\right)\frac{x_{j+1}-x}{h_j}+\left(y_{j+1}-\frac{M_{j+1}h_j^2}{6}\right)\frac{x-x_j}{h_j},\ \ j=0,1,\cdots,n-1$$

$\mu_jM_{j-1}+2M_j+\lambda_jM_{j+1}=d_j$，$j=1,2,\cdots,n-1$，

$\boldsymbol{\mu_j}=\frac{\boldsymbol{h_{j-1}}}{\boldsymbol{h_{j-1}+h_j}}$，$\boldsymbol{\lambda_j}=\frac{\boldsymbol{h_j}}{\boldsymbol{h_{j-1}+h_j}}$，$j=1,2,\cdots,n-1$，

$d_j=6\frac{f[x_j,x_{j+1}]-f[x_{j-1},x_j]}{h_{j-1}+h_j}=6f\left[x_{j-1},x_j,x_{j+1}\right]$

第一种边界条件：$S'(x_0)=f_0'$，$S'(x_n)=f_n'$

$2M_0+M_1=\frac{6}{h_0}(f[x_0,x_1]-f_0')\ M_{n-1}+2M_n=\frac{6}{h_{n-1}}(f_n'-f[x_{n-1},x_n])$

令 $\boldsymbol{\lambda_0=1}, d_0=\frac{6}{h_0}(f[x_0,x_1]-f_0'), \boldsymbol{\mu_n=1}, d_n=\frac{6}{h_{n-1}}(f_n'-f[x_{n-1},x_n])$ 则矩阵形式为：

$$\begin{pmatrix}2&\lambda_0&&&\\\mu_1&2&\lambda_1&&\\&\ddots&\ddots&\ddots&\\&&\mu_{n-1}&2&\lambda_{n-1}\\&&&\mu_n&2\end{pmatrix}\begin{pmatrix}M_0\\M_1\\\vdots\\M_{n-1}\\M_n\end{pmatrix}=\begin{pmatrix}d_0\\d_1\\\vdots\\d_{n-1}\\d_n\end{pmatrix}$$

第二种边界条件：$S''(x_0)=f_0''$，$S''(x_n)=f_n''$

$\boldsymbol{M_0=f_0'', M_n=f_n''}, \lambda_0=\mu_n=0, d_0=2f_0'', d_n=2f_n''$

03 逼近与拟合

无穷范数：$\|f\|_\infty=\max_{a\leq x\leq b}|f(x)|$

1 范数：$\|f\|_1=\int_a^b|f(x)|\,dx$ 2 范数：$\|f\|_2=\left(\int_a^bf(x)^2\,dx\right)^{\frac12}$

(u,v) 为 X(X 是 R 或 C 上的线性空间)上的**内积**：

$(u,v)=\overline{(v,u)},\quad\forall u,v\in X$;

$(\alpha u,v)=\alpha(v,u),\forall\alpha\in K,\ \forall u,v\in X$;

$(u+v,w)=(u,w)+(v,w),\ \forall u,v,w\in X$;

$(u,u)\geq0$; *if and only if* $\mathbf{u}=\mathbf{0},(\mathrm{u},\mathrm{u})=0$

柯西-施瓦茨不等式：$|(u,v)|^2\leq(u,u)(v,v)$

带权内积与范数：

$x,y\in R^n,\rho_i>0$，$(x,y)=\sum_{i=1}^n\boldsymbol{\rho_i}x_iy_i$，$||x||_2=\left(\sum_{i=1}^n\rho_ix_i^2\right)^{\frac12}$

$f(x),g(x)\in C[a,b]$，$(f(x),g(x))=\int_a^b\boldsymbol{\rho(x)}f(x)g(x)\mathrm{d}x$

$\|f(x)\|_2=(f(x),f(x))^{1/2}=\left[\int_a^b\boldsymbol{\rho(x)}f^2(x)\mathrm{d}x\right]^{1/2}$

$$G=\begin{bmatrix}(u_1,u_1)&(u_2,u_1)&\cdots&(u_n,u_1)\\(u_1,u_2)&(u_2,u_2)&\cdots&(u_n,u_2)\\\vdots&\vdots&\cdots&\vdots\\(u_1,u_n)&(u_2,u_n)&\cdots&(u_n,u_n)\end{bmatrix}$$

Gram 矩阵，非奇异的充要条件是 $u_1,u_2,\ldots u_n$ 线性无关

最佳一致逼近多项式：$\|f(x)-P^*(x)\|_\infty$

$=\min_{P\in H_n}\|f(x)-P(x)\|_\infty=\min_{P\in H_n}\max_{a\leq x\leq b}|f(x)-P(x)|$

最佳平方逼近多项式：$\|f(x)-P^*(x)\|_2^2$

$=min_{P\in H_n}\|f(x)-P(x)\|_2^2=\min_{P\in H_n}\int_a^b|f(x)-P(x)|^2dx$

最小二乘拟合：$\sum_{i=0}^m|y_i-g^*(x_i)|^2=\min_{g\in\Phi}\sum_{i=0}^m|y_i-g(x_i)|^2$

最佳平方逼近函数：最小化 $I(a_0,a_1,\cdots,a_n)$ 的问题

$I(a_0,a_1,\cdots,a_n)=\int_a^b\rho(x)[\sum_{j=0}^na_j\phi_j-f(x)]^2\mathrm{d}x$

$\frac{\partial I(a_0,\cdots,a_n)}{\partial a_k}=2\int_a^b\rho(x)[\sum_{j=0}^na_j\phi_j(x)-f(x)]\phi_k(x)\mathrm{d}x=0$

$\sum_{j=0}^n(\phi_j(x),\phi_k(x))a_j=(f(x),\phi_k(x))(k=0,1,\cdots,n)$

$$\begin{bmatrix}(\phi_0,\phi_0)&(\phi_0,\phi_1)&\cdots&(\phi_0,\phi_n)\\(\phi_1,\phi_0)&(\phi_1,\phi_1)&\cdots&(\phi_1,\phi_n)\\\vdots&\vdots&\cdots&\vdots\\(\phi_n,\phi_0)&(\phi_n,\phi_1)&\cdots&(\phi_n,\phi_n)\end{bmatrix}\begin{bmatrix}a_0\\a_1\\\vdots\\a_n\end{bmatrix}=\begin{bmatrix}(f,\phi_0)\\(f,\phi_1)\\\vdots\\(f,\phi_n)\end{bmatrix}$$

误差：$\|\delta(x)\|_2^2=\|f(x)\|_2^2-\sum_{k=0}^na_k^*(\phi_k(x),f(x))$

例题：$f(x)=\sqrt{x},x\in\left[\frac14,1\right],\phi=span\{1,x\},\rho(x)=1$

已知 $\phi_0=1,\phi_1=x$，设所求 $S_1^*(x)=a_0+a_1x$，法方程：

$\begin{bmatrix}(\phi_0,\phi_0)&(\phi_0,\phi_1)\\(\phi_1,\phi_0)&(\phi_1,\phi_1)\end{bmatrix}\begin{bmatrix}a_0\\a_1\end{bmatrix}=\begin{bmatrix}(f,\phi_0)\\(f,\phi_1)\end{bmatrix}$ $(\phi_0,\phi_0)=\int_{\frac14}^1\mathrm{d}x=\frac34$,

$(\phi_1,\phi_1)=\int_{\frac14}^1x^2\mathrm{d}x=\frac{21}{64}$ $(f,\phi_0)=\int_{\frac14}^1\sqrt{x}\mathrm{d}x=\frac{7}{12}$

$(\phi_1,\phi_0)=(\phi_0,\phi_1)=\int_{\frac14}^1x\mathrm{d}x=\frac{15}{32}$ $(f,\phi_1)=\int_{\frac14}^1x\sqrt{x}\mathrm{d}x=\frac{31}{80}$

$\begin{bmatrix}\frac34&\frac{15}{32}\\\frac{15}{32}&\frac{21}{64}\end{bmatrix}\begin{bmatrix}a_0\\a_1\end{bmatrix}=\begin{bmatrix}\frac{7}{12}\\\frac{31}{80}\end{bmatrix},\Rightarrow\begin{cases}a_0=\frac{10}{27},\\a_1=\frac{88}{135}.\end{cases}\quad S_1^*(x)=\frac{10}{27}+\frac{88}{135}x.$

误差 $\|\delta(x)\|_2^2=\int_{\frac{1}{4}}^{1} x\mathrm{d}x-\left(\frac{10}{27}\times\frac{7}{12}+\frac{31}{80}\times\frac{88}{135}\right)=0.0001082$

希尔伯特矩阵：$\varphi_k(x)=x^k,\rho(x)\equiv 1,f(x)\in C[0,1]$,
求 n 次最佳平方逼近多项式：$S_n^*(x)=a_0^*P_0(x)+a_1^*P_1(x)+$

$\cdots+a_n^*P_n(x)$, 此时 $\left(\varphi_j(x),\varphi_k(x)\right)=\int_0^1 x^{k+j}\mathrm{d}x=\frac{1}{k+j+1}$,

$(f(x),\varphi_k(x))=\int_0^1 f(x)x^k\mathrm{d}x\equiv d_k$ 称 H 为希尔伯特(Hilbert)

矩阵，记 $a=(a_0,a_1,\cdots,a_n)^{\mathrm{T}}$，$d=(d_0,d_1,\cdots,d_n)^{\mathrm{T}}$

$Ha=d$ 的解 $a_k=a_k^*(k=0,1,\cdots,n)$ 即为所求

$$\mathbf{H}=\begin{bmatrix}1 & 1/2 & \cdots & 1/(n+1)\\ 1/2 & 1/3 & \cdots & 1/(n+2)\\ \vdots & \vdots & & \vdots\\ 1/(n+1) & 1/(n+2) & \cdots & 1/(2n+1)\end{bmatrix}$$

曲线拟合的最小二乘法：$(\phi_k,\phi_j)=\sum_{i=0}^m \rho(x_i)\phi_k(x_i)\phi_j(x_i)$
$(f,\phi_j)=\sum_{i=0}^m \rho(x_i)f(x_i)\phi_j(x_i)$

$\|\partial\|_2=[\|y\|_2^2-a(\varphi_0,y)-b(\varphi_1,y)]^{1/2}$

总结：最佳平方逼近是**求积分**，最小二乘法是**求加权和。**

Schemite 正交化：$f_0(x),f_1(x),f_2(x)\ldots f_n(x)$ 线性无关

$g_0(x)=f_0(x)$, $g_1(x)=f_1(x)-\frac{(f_1,g_0)}{(g_0,g_0)}g_0(x)$

$g_n(x)=f_n(x)-\sum_{i=0}^{n-1}\frac{(f_n,g_i)}{(g_i,g_i)}g_i(x)$ 则 g 为正交多项式

其中 f 为 $1,x,x^2,x^3,\ldots x^n$ 区间[-1,1]，$\rho(x)=1$, Legendre

正交多项式的性质：$(f(x),g(x))=\int_a^b \rho(x)f(x)g(x)\mathrm{d}x=0$

$(\varphi_j,\varphi_k)=\int_a^b \rho(x)\varphi_j(x)\varphi_k(x)\mathrm{d}x=\begin{cases}0, & j\neq k,\\ A_k>0, & j=k.\end{cases}$

勒让德多项式：$[-1,1]$，$\rho(t)=1$，$P_0(t)=1$, $P_1(t)=t$,

$(k+1)P_{k+1}(t)=(2k+1)tP_k(t)-kP_{k-1}(t),k=1,2,\ldots$

切比雪夫 1：$[-1,1]$，$\rho(t)=\frac{1}{\sqrt{1-t^2}}$，$T_0(t)=1$，$T_1(t)=t$,

$T_{k+1}(t)=2tT_k(t)-T_{k-1}(t),k=1,2,\cdots$

切比雪夫 2：$[-1,1]$，$\rho(t)=\sqrt{1-t^2}$，$U_0(t)=1$，$U_1(t)=2t$,

$U_{k+1}(t)=2tU_k(t)-U_{k-1}(t)$，$k=1,2,\cdots$

拉盖尔：$[0,+\infty]$, $\rho(t)=e^{-t}$，$L_0(t)=1$, $L_1(t)=1-t$,

$L_{k+1}(t)=(1+2k-t)L_k(t)-k^2L_{k-1}(t)$，$k=1,2,\cdots$

埃尔米特：$(-\infty,+\infty)$，$\rho(t)=e^{-t^2}$, $H_0(t)=1$, $H_1(t)=2t$

$H_{k+1}(t)=2tH_k(t)-2kH_{k-1}(t)$，$k=1,2,\cdots$

最佳平方逼近：$S^*(x)=\sum_{k=0}^n\frac{(f(x),\varphi_k(x))}{(\varphi_k(x),\varphi_k(x))}\varphi_k(x),k=0,1,\cdots,n.$

误差：$\|\delta_n(x)\|_2=\|f(x)-S_n^*(x)\|_2=\left(\|f(x)\|_2^2-\sum_{k=0}^n\left[\frac{(f(x),\phi_k(x))}{\|\phi_k(x)\|_2}\right]^2\right)^{\frac{1}{2}}$

勒让德逼近：$f(x)\in C[-1,1]$，按 $P_0(x),P_1(x),\ldots,P_n(x)$ 展开
$S_n^*(x)=a_0^*P_0(x)+a_1^*P_1(x)+\cdots+a_n^*P_n(x)$, $P_0(x)=1$,
$P_1(x)=x$，$P_2(x)=(3x^2-1)/2$, $P_3(x)=(5x^3-3x)/2$,
$P_4(x)=(35x^4-30x^2+3)/8$

系数：$a_k^*(x)=\frac{(f(x),P_k(x))}{(P_k(x),P_k(x))}=\frac{2k+1}{2}\int_{-1}^1 f(x)P_k(x)dx$

平方逼近误差：$\|\delta_k(x)\|_2^2=\int_{-1}^1 f^2(x)dx-\sum_{k=0}^n\frac{2}{2k+1}a_k^{*2}$

04a 数值积分

如果某个求积公式对于次数不超过 m 的多项式均能准确地成立，但对于 m+1 次的多项式就不准确成立，则称该求积公式具有 **m 次代数精度。**

$\int_0^1 f(x)dx\approx Af(0)+Bf(x_1)+Cf(1)$

令 $f(x)=1,x,x^2,x^3$ 左边等于右边 四个未知数四个方程

插值型的求积公式：$I_n=\int_a^b L_n(x)dx=$

$\int_a^b\sum_{k=0}^n l_k(x)f_k\,dx=\sum_{k=0}^n\left[\int_a^b l_k(x)dx\right]f_k=\sum_{k=0}^n A_k f_k$

余项为 $R[f]=I-I_n=\int_a^b[f(x)-L_n(x)]\,dx=$

$\int_a^b\frac{f^{(n+1)}(\xi)}{(n+1)!}\omega_{n+1}(x)\,dx$，Ln 为拉格朗日插值。

$\frac{1}{b-a}\int_a^b f(x)dx=f(c)$, $g(x)\geq 0$

积分中值定理：$\int_a^b f(x)g(x)dx=f(c)\int_a^b g(x)dx$

牛顿-柯特斯公式：[a,b] n 等分,步长 $h=\frac{b-a}{n}$

等距节点 $x_k=a+kh$, $I_n=(b-a)\sum_{k=0}^n C_k^{(n)}f(x_k)$

$A_k=\int_a^b l_k(x)dx,k=0,1,\cdots,n$ 令 $x=a+th$

$$C_k^{(n)}=\frac{h}{b-a}\int_0^n\prod_{j=0,j\neq k}^n\frac{t-j}{k-j}dt=\frac{(-1)^{n-k}}{nk!\,(n-k)!}\int_0^n\prod_{j=0,j\neq k}^n(t-j)dt$$

梯形公式(n=1)：

$$\int_a^b f(x)dx\approx T=\frac{b-a}{2}[f(a)+f(b)]$$

$$R[f]=\frac{1}{2!}\int_a^b f''(\xi_x)(x-a)(x-b)dx$$

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

辛普森公式(n=2)：

$$\int_a^b f(x)\,dx\approx S=\frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]$$

$$R[f]=-\frac{b-a}{180}\left(\frac{b-a}{2}\right)^4f^{(4)}(\eta)=-\frac{(b-a)^5}{2880}f^{(4)}(\eta)$$

牛顿-柯特斯公式(n=4)：

$\int_a^b f(x)\,dx\approx C=\frac{b-a}{90}[7f(x_0)+32f(x_1)+12f(x_2)+$

$32f(x_3)+7f(x_4)]$，其中 $x_k=a+kh,h=\frac{b-a}{4}$

$$R[f]=-\frac{2(b-a)}{945}\left(\frac{b-a}{4}\right)^6 f^{(6)}(\eta)=-\frac{(b-a)^7}{1935360}f^{(6)}(\eta)$$

n/k	0	1	2	3	4	5	6
1	$\frac{1}{2}$	$\frac{1}{2}$					
2	$\frac{1}{6}$	$\frac{4}{6}$	$\frac{1}{6}$				
3	$\frac{1}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{1}{8}$			
4	$\frac{7}{90}$	$\frac{16}{45}$	$\frac{2}{15}$	$\frac{16}{45}$	$\frac{7}{90}$		
5	$\frac{19}{288}$	$\frac{25}{96}$	$\frac{25}{144}$	$\frac{25}{144}$	$\frac{25}{96}$	$\frac{19}{288}$	
6	$\frac{41}{840}$	$\frac{9}{35}$	$\frac{9}{280}$	$\frac{34}{105}$	$\frac{9}{280}$	$\frac{9}{35}$	$\frac{41}{840}$

$$R[f]=\begin{cases}\dfrac{f^{(n+1)}(\eta)}{(n+1)!}\displaystyle\int_a^b \omega_{n+1}(x)dx & (n\text{ 为奇数})\\ \dfrac{f^{(n+2)}(\eta)}{(n+2)!}\displaystyle\int_a^b x\omega_{n+1}(x)dx & (n\text{ 为偶数})\end{cases}$$

复合梯形公式：$x_k=a+kh,\ h=\frac{b-a}{n},k=0,1,\dots n-1$

$$I=\int_a^b f(x)dx=\sum_{k=0}^{n-1}\int_{x_k}^{x_{k+1}}f(x)dx=\sum_{k=0}^{n-1}\frac{\mathbf{h}}{\mathbf{2}}[\mathbf{f(x_k)}+\mathbf{f(x_{k+1})}]+R_n[f]$$

$$T_n=\frac{\mathbf{h}}{\mathbf{2}}\sum_{k=0}^{n-1}[\mathbf{f(x_k)}+\mathbf{f(x_{k+1})}]=\frac{h}{2}\left[f(a)+2\sum_{k=1}^{n-1}f(x_k)+f(b)\right]$$

$$R_n[f]=I-T_n=\sum_{k=0}^{n-1}\left[-\frac{h^3}{12}f''(\eta_k)\right]=-\frac{b-a}{12}h^2f''(\eta)$$

$$f''(\xi)=\frac{1}{n}[f''(\xi_1)+f''(\xi_2)+\cdots f''(\xi_n)]\text{ 介值定理}$$

$$\lim_{h\to 0}\frac{\int_a^b f(x)dx-T_n}{h^2}=\lim_{h\to 0}\left(-\frac{1}{12}\sum_{k=1}^{n}f''(\xi_k)h\right)$$

$$=-\frac{1}{12}\int_a^b f''(x)dx=-\frac{1}{12}[f'(b)-f'(a)]$$

复合辛普森公式：$I=\int_a^b f(x)dx=\sum_{k=0}^{n-1}\frac{h}{6}\left[f(x_k)+4f\left(x_{k+\frac{1}{2}}\right)+f(x_{k+1})\right]+R_n[f]$，$x_{k+\frac{1}{2}}$ 为$[x_k,x_{k+1}]$中点

$$S_n=\frac{h}{6}\sum_{k=0}^{n-1}\left[f(x_k)+4f\left(x_{k+\frac{1}{2}}\right)+f(x_{k+1})\right]$$

$$=\frac{h}{6}\left[f(a)+4\sum_{k=0}^{n-1}f(x_{k+\frac{1}{2}})+2\sum_{k=1}^{n-1}f(x_k)+f(b)\right]$$

$$R_n[f]=I-S_n=-\frac{h}{180}\left(\frac{h}{2}\right)^4\sum_{k=0}^{n-1}f^{(4)}(\eta_k)=-\frac{b-a}{180}\left(\frac{h}{2}\right)^4 f^{(4)}(\eta)$$

龙贝格求积公式：对**复合公式**做四则运算 $\frac{I-T_n}{I-T_{2n}}\approx 4$

$$T_{2n}=\sum_{k=0}^{n-1}\frac{1}{2}\left(\frac{h}{2}\right)\left[f(x_k)+2f\left(x_{k+\frac{1}{2}}\right)+f(x_{k+1})\right]\quad h=(b-a)/n$$

$$=\frac{h}{4}\sum_{k=0}^{n-1}[f(x_k)+f(x_{k+1})]+\frac{h}{2}\sum_{k=0}^{n-1}f(x_{k+\frac{1}{2}})=\frac{1}{2}T_n+\frac{h}{2}\sum_{k=0}^{n-1}f(x_{k+\frac{1}{2}})$$

$$I-T_n=-\frac{b-a}{12}h^2f''(\eta_1)\ \eta_1\in(a,b)\quad I-T_{2n}=-\frac{b-a}{12}\left(\frac{h}{2}\right)^2 f''(\eta_2)\ \eta_2\in(a,b)$$

$$S_n=\frac{4T_{2n}-T_n}{4-1},\quad C_n=\frac{4^2S_{2n}-S_n}{4^2-1},\quad R_n=\frac{4^3C_{2n}-C_n}{4^3-1}$$

k	h	$T_0^{(k)}$	$T_1^{(k)}$
0	$b-a$	$T_0^{(0)}$	
1	$\frac{b-a}{2}$	$T_0^{(1)}$ ↓①	$T_1^{(0)}$
2	$\frac{b-a}{4}$	$T_0^{(2)}$ ↓②	$T_1^{(1)}$ ↓③

高斯求积公式：选取高斯点有 2n+1 次代数精度

$$\int_a^b x^m\rho(x)dx=\sum_{i=0}^{n}A_ix_i^m,m=0,1,\cdots,2n+1$$

插值节点是**高斯点**⇔与任何不超过 n 次的多项式 $P(x)$ 带权 $\rho(x)$ 正交：$\int_a^b\rho(x)\omega_{n+1}(x)P(x)dx=0$

定理：权函数为 $\rho(x)$ 的积分 $I=\int_a^b f(x)\rho(x)dx$, 区间 [a,b] 上权函数为 $\rho(x)$ 的**正交多项式** $p_n(x)$ 的 **n 个零点**恰为 Gauss 点。一般选 $1,x,x^2,\dots x^n$

计算积分系数：$A_i=\int_a^b l_i(x)\rho(x)dx\ (i=1,2,\dots n)$

Schemite 正交化：$(f(x),g(x))=\int_a^b\rho(x)f(x)g(x)dx$

$$p_0(x)=1,\qquad p_1(x)=x-\frac{(x,p_0(x))}{(p_0(x),p_0(x))}p_0(x)$$

$$p_2(x)=x^2-\frac{(x^2,p_0(x))}{(p_0(x),p_0(x))}p_0(x)-\frac{(x^2,p_1(x))}{(p_1(x),p_1(x))}p_1(x)$$

Gauss-Legendre 求积公式：[-1,1]，$\rho(x)=1$

$$\int_{-1}^1 f(x)dx\approx\sum_{k=0}^{n}A_kf(x_k)$$

$$R[f]=\frac{2^{2n+1}(n!)^4}{[(2n)!]^3(2n+1)}f^{(2n)}(\eta),\eta\in(-1,1)$$

n	xk	Ak	n	xk	Ak
0	0	2	3	±0.861 1363, ±0.339 9810	0.347 8548, 0.652 1452
1	±0.577 3503	1	4	±0.906 1798, ±0.538 9463, 0	0.236 9269, 0.478 6287, 0.568 8889,
2	±0.774 5967, 0	0.555 5556, 0.888 8889	5	±0.932 4695, ±0.661 2094, ±0.238 6192	0.171 3245, 0.360 7616, 0.467 9139

当区间为[a,b]时，做变换 $x=\frac{b-a}{2}t+\frac{a+b}{2}$

可将[a,b]化为[-1,1]，此时

$$\int_a^b f(x)dx=\frac{b-a}{2}\int_{-1}^1 f\left(\frac{b-a}{2}t+\frac{a+b}{2}\right)dt$$

$$\approx \frac{b-a}{2}\sum_{i=1}^{n} A_i f\left(\frac{a+b}{2}+\frac{b-a}{2}x_i\right)$$

此时 $R[f]=\frac{(b-a)^{2n+1}(n!)^4}{[(2n)!]^3(2n+1)}f^{(2n)}(\eta),\eta\in(a,b)$

Gauss-Laguerre：$\int_0^{+\infty} e^{-x}f(x)\,d\,x \approx \sum_{k=0}^{n} A_k f(x_k)$

n	x_k	A_k
0	1	1
1	0.585 786 438 3.414 213 562	0.853 553 391 0.146 446 609
2	0.415 774 557 2.294 280 360 6.289 945 083	0.711 093 010 0.278 517 734 0.010 389 257
3	0.322 547 690 1.745 761 101 4.536 620 297 9.395 070 912	0.603 154 104 0.357 418 692 0.038 887 909 0.000 539 295

Gauss-Hermite：$\int_{-\infty}^{+\infty} e^{-x^2}f(x)\,d\,x \approx \sum_{k=0}^{n} A_k f(x_k)$

n	x_k	A_k
0	0	1.772 453 851
1	±0.707 106 781	0.886 226 926
2	±1.224 744 871 0	0.295 408 975 1.181 635 901
3	±1.650 680 124 ±0.524 647 623	0.081 312 835 0.804 914 090
4	±2.020 182 871 ±0.958 572 465 0	0.019 953 242 0.393 619 323 0.945 308 721

04b 数值微分

向前差商公式：$f'(x)\approx\frac{f(x+h)-f(x)}{h}-\frac{h}{2}f''(\xi)$

向后差商公式：$f'(x)\approx\frac{f(x)-f(x-h)}{h}+\frac{h}{2}f''(\xi)$

中心差商公式：$f'(x)\approx\frac{f(x+h)-f(x-h)}{2h}-\frac{h^2}{6}f^{(3)}(\xi)$

$$E(f,h)=E_{round}(f,h)+E_{trunc}(f,h)$$

$=\frac{e_1-e_{-1}}{2h}-\frac{h^2f^{(3)}(c)}{6}\le\frac{\varepsilon}{h}+\frac{h^2}{6}M$ 所以 h 不能太小

插值型的求导公式：$f'(x)\approx P_n'(x)$

$$f'(x)-P_n'(x)=\frac{f^{(n+1)}(\xi)}{(n+1)!}\omega_{n+1}'(x)+\frac{\omega_{n+1}(x)}{(n+1)!}\frac{d}{dx}f^{(n+1)}(\xi)$$

$\boldsymbol{\omega_{n+1}(x_k)=0}$ 则 $f'(x_k)-P_n'(x_k)=\frac{f^{(n+1)}(\xi)}{(n+1)!}\omega_{n+1}'(x_k)$

例：拉格朗日插值三点式

$f(x)=L_{i-1}(x)f(x_{i-1})+L_i(x)f(x_i)+L_{i+1}(x)f(x_{i+1})=$

$f(x_{i-1})\frac{(x-x_i)(x-x_{i+1})}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})}+f(x_i)\frac{(x-x_{i-1})(x-x_{i+1})}{(x_i-x_{i-1})(x_i-x_{i+1})}+f(x_{i+1})\frac{(x-x_{i-1})(x-x_i)}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)}$

$f'(x)=f(x_{i-1})\frac{2x-x_i-x_{i+1}}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})}+f(x_i)\frac{2x-x_{i-1}-x_{i+1}}{(x_i-x_{i-1})(x_i-x_{i+1})}$

$+f(x_{i+1})\frac{2x-x_{i-1}-x_i}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)}$ 代入 x_{i-1},x_i,x_{i+1} 可得

Forward: $f'(x_{i-1})=\frac{-3f(x_{i-1})+4f(x_i)-f(x_{i+1})}{2h}+\frac{h^2}{3}f^{(3)}(\xi)$

Centered: $f'(x_i)=\frac{f(x_{i+1})-f(x_{i-1})}{2h}-\frac{h^2}{6}f^{(3)}(\xi)$

Backward: $f'(x_{i+1})=\frac{f(x_{i-1})-4f(x_i)+3f(x_{i+1})}{2h}+\frac{h^2}{3}f^{(3)}(\xi)$

05 解线性方程组的直接法

列主元消去法：选择**绝对值最大**的元素作为主元

直接三角分解法：L 的元素是下行减去上行的系数

$\begin{matrix} L_{n-1}\cdots L_2L_1A^{(1)}=A^{(n)} \\ L_{n-1}\cdots L_2L_1b^{(1)}=b^{(n)} \end{matrix}$ $A=L_1^{-1}L_2^{-1}\cdots L_{n-1}^{-1}U=LU$

Ax=b 等价于 $Ly=b,Ux=y$，$Ax=LUx=L(Ux)=Ly=b$

$$A=\begin{bmatrix}1&2&3\\2&5&2\\3&1&5\end{bmatrix}=\begin{bmatrix}1&0&0\\2&1&0\\3&-5&1\end{bmatrix}\begin{bmatrix}1&2&3\\0&1&-4\\0&0&-24\end{bmatrix}=LU$$

平方根法：设 A 为对称正定矩阵，Cholesky 分解：

$$D^{\frac{1}{2}}=\begin{pmatrix}\sqrt{u_{11}}&&&\\&\sqrt{u_{22}}&&\\&&\ddots&\\&&&\sqrt{u_{nn}}\end{pmatrix}$$

$$\begin{bmatrix}2&-1&1\\-1&-2&3\\1&3&1\end{bmatrix}=\begin{bmatrix}1&&\\l_{21}&1&\\l_{31}&l_{32}&1\end{bmatrix}\begin{bmatrix}d_1&&\\&d_2&\\&&d_3\end{bmatrix}\begin{bmatrix}1&l_{21}&l_{31}\\&1&l_{32}\\&&1\end{bmatrix}$$

$A=LD^{\frac{1}{2}}D^{\frac{1}{2}}L^{T}=(LD^{\frac{1}{2}})(LD^{\frac{1}{2}})^{T}=GG^{T}$ 其中,$G=LD^{\frac{1}{2}}$

追赶法：矩阵须满足对角占优条件，$|b_1|>|c_1|>0,|b_n|>|a_n|>0,|b_i|\ge|a_i|+|c_i|$

$$\begin{bmatrix}b_1&c_1&&&\\a_2&b_2&c_2&&\\&\ddots&\ddots&\ddots&\\&&a_{n-1}&b_{n-1}&c_{n-1}\\&&&a_n&b_n\end{bmatrix}\begin{bmatrix}x_1\\x_2\\\vdots\\x_{n-2}\\x_{n-1}\\x_n\end{bmatrix}=\begin{bmatrix}f_1\\f_2\\\vdots\\f_{n-1}\\f_n\end{bmatrix}$$

$$A=\begin{bmatrix}\alpha_1&&&\\\gamma_2&\alpha_2&&\\&\ddots&\ddots&\\&&\gamma_n&\alpha_n\end{bmatrix}\begin{bmatrix}1&\beta_1&&\\&1&\ddots&\\&&\ddots&\beta_{n-1}\\&&&1\end{bmatrix}=LU$$

$\beta_1=c_1/b_1$，$\beta_i=c_i/(b_i-a_i\beta_{i-1})$ $(i=2,3,\dots,n-1)$，
$\alpha_1=b_1$，$\alpha_i=b_i-a_i\beta_{i-1}$ $(i=2,3,\dots n)$，$\gamma_i=a_i$

解 $Ly=f$：$y_1=f_1/b_1$，

$y_i = (f_i - a_i y_{i-1})/(b_i - a_i\,\beta_{i-1})\ \ (i = 2,3,\dots n)$

解 $Ux = y$：$x_n = y_n$，

$x_i = y_i - \beta_i x_{i+1}\ \ (i = n-1, n-2, \dots 2,1)$

向量范数：正定($||x|| \ge 0$)；齐次($||kx|| = |k|||x||$)；

三角不等式。无穷范数：$\| x \|_\infty = \max\limits_{1\le i\le n}|x_i|$

P 范数：$\|x\|_p = \left(\sum_{i=1}^{n} x_i^2\right)^{\frac{1}{p}}$ **谱半径** $\rho(A) = \max\limits_{1\le i\le n}|\lambda_i|$

矩阵范数：$\|A\|_\infty = \max\limits_{1\le i\le n}\sum_{j=1}^{n}|a_{ij}|$ 矩阵的行范数

$\|A\|_1 = \max\limits_{1\le j\le n}\sum_{i=1}^{n}|a_{ij}|$ 矩阵的列范数

$\|A\|_2 = \sqrt{\lambda_{max}(A^{\mathrm{T}}A)}$ 矩阵的 2-范数(谱范数)

$\| A \|_{\mathrm{F}} = \sqrt{\sum_{i,j=1}^{n} a_{ij}^2}$ 矩阵的 F-范数

06 解线性方程组的迭代法

雅可比迭代法：$x^{(0)} = \left(x_1^{(0)}, \cdots, x_n^{(0)}\right)^{\mathrm{T}}$

$x_i^{(k+1)} = (b_i - \sum_{j=1,j\ne i}^{n} a_{ij}x_j^{(k)})/a_{ii}, (i = 1, \cdots, n)$

高斯-赛德尔迭代法：$x_i^{(k+1)} = x_i^{(k)} + \Delta x_i$

$\Delta x_i = \left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(k+1)} - \sum_{j=i}^{n} a_{ij}x_j^{(k)}\right)/a_{ii}$ 或

$x_i^{(k+1)} = \left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(k+1)} - \sum_{j=i+1}^{n} a_{ij}x_j^{(k)}\right)/a_{ii}$

超松驰(Successive Over-Relaxation)迭代法：

$x_i^{(k+1)} = x_i^{(k)} + \omega\Delta x_i\ \ 0 < \omega < 2$ 收敛

$x_i^{(k+1)} = x_i^{(k)} + \omega\left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(k+1)} - \sum_{j=i}^{n} a_{ij}x_j^{(k)}\right)/a_{ii}$ $\omega = 1$，高斯－赛德尔迭代；

$1 < \omega < 2$，超松弛法；$\omega < 1$，低松弛法；

迭代法的收敛性：$A = D - L - U$ 初值取全 1 或全 0

$$D = \begin{bmatrix} a_{11} & & & \\ & a_{22} & & \\ & & \ddots & \\ & & & a_{nn} \end{bmatrix} \quad L = \begin{bmatrix} 0 & & & \\ -a_{21} & 0 & & \\ \vdots & \ddots & \ddots & \\ -a_{n1} & \cdots & -a_{n,n-1} & 0 \end{bmatrix}$$

$$U = \begin{bmatrix} 0 & -a_{12} & \cdots & -a_{1n} \\ & 0 & \ddots & \vdots \\ & & \ddots & -a_{n-1,n} \\ & & & 0 \end{bmatrix}$$

$x^{(k+1)} = Bx^k + f$ 收敛的充要条件是谱半径 $\rho(B) < 1$

雅可比迭代法：$B_J = D^{-1}(L+U), f_J = D^{-1}b$;

高斯-赛德尔迭代法：$B_G = (D-L)^{-1}U, f_G = (D-L)^{-1}b$ SOR 迭代法：$B_G = (D-\omega L)^{-1}[(1-\omega)D + \omega U]$，$f_S = \omega(D-\omega L)^{-1}b$

严格对角占优：$\sum_{j=1,j\ne i}^{n}|a_{ij}| < |a_{ii}|$ 则高斯/雅可比收敛

若 A 为对称正定矩阵且 $0 < \omega < 2$，则 SOR 收敛

若 A 严格对角占优且 $0 < \omega \le 1$，则 SOR 收敛

07 非线性方程（组）求根

方程求根与二分法：$f(x) = (x-\alpha)^m h(x), f(\alpha) = f'(\alpha) = \cdots = f^{m-1}(\alpha) = 0$，$f^m(\alpha) \ne 0$ 则 α 是 m 重零点

$| x_k - x^* | \le (b_k - a_k)/2 = (b-a)/2^{k+1}\ \ k = 0, 1, 2\dots$

$x_k = (a_k + b_k)/2 \to x^*$ (当 $k \to \infty$ 时)

二分法表格表头：$k, a_k, b_k, x_k, f(x_k)$的符号

迭代法：$x_{k+1} = \phi(x_k)$，$k = 0,1,2,\cdots$

存在唯一的不动点：$\forall x \in [a,b]\ \ \phi(x) \in [a,b]$; (1)

$|\phi(x) - \phi(y)| \le L|x-y|\quad 0 \le L < 1$ (2)

条件(2)可变为 $|\boldsymbol{\phi'(x)}| \le \boldsymbol{L} < \boldsymbol{1}$

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

局部收敛性与收敛阶: 误差 $e_k = x_k - x^*$

若 $lim_{k\to\infty}\frac{e_{k+1}}{e_k^p} = C, C \ne 0$, 则 p 阶收敛

p=1 线性，p>1 超线性，p=2 平方收敛

$\phi'(x^*) = \phi''(x^*) = \cdots = \phi^{(p-1)}(x^*) = 0, \phi^{(p)}(x^*) \ne 0$, p 阶收敛

$0 < |\phi'(x^*)| < 1$, 线性; $|\phi'(x^*)| = 0, |\phi''(x^*)| \ne 0$ 平方收敛

Aitken 迭代法：$\hat{x}_k = x_k - \frac{(x_{k+1} - x_k)^2}{x_{k+2} - 2x_{k+1} + x_k}$

Steffenson 迭代法：$y_k = \phi(\mathrm{x_k})$，$z_k = \phi(y_k)$

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

牛顿法：求 f(x) = 0 的根： $x_{k+1}=x_k-\frac{f(x_k)}{f'(x_k)}\ \ f'(x_k)\neq 0$

$$0=f(x^*)=f(x_k)+f'(x_k)(x^*-x_k)+\frac{f''(\xi_k)}{2}(x^*-x_k)^2$$

$$0=x^*+\frac{f(x_k)}{f'(x_k)}-x_k+\frac{f''(\xi_k)}{2f'(x_k)}(x^*-x_k)^2$$

$$0=x^*-x_{k+1}+\frac{f''(\xi_k)}{2f'(x_k)}(x^*-x_k)^2$$

$$\lim_{k\to\infty}\frac{x_{k+1}-x^*}{(x_k-x^*)^2}=\lim_{k\to\infty}\frac{f''(\xi_k)}{2f'(x_k)}=\frac{f''(x^*)}{2f'(x^*)}$$

$\phi'(x)=\frac{f(x)f''(x)}{[f'(x)]^2}$， $f(x^*)=0$， $\phi''(x^*)=$

$\frac{[f'(x^*)f''(x^*)+0f'''(x^*)][f'(x^*)]^2-0}{[f'(x^*)]^4}=\frac{f''(x^*)}{f'(x^*)}$

当 x^* 是 $f(x)$ 的单根时, $\phi'(x^*)=0,\phi''(x^*)\neq 0$ 平方收敛

m 重根情形, $f(x)=(x-\alpha)^m h(x)$, 牛顿法不是平方收敛

可将迭代法改为 $x_{k+1}=x_k-m\frac{f(x_k)}{f'(x_k)}$, 仍平方收敛

法二：令 $F(x)=[f(x)]^{\frac{1}{m}}=(x-\alpha)[h(x)]^{\frac{1}{m}}$

$\mu(x)=\frac{(x-\alpha)h(x)}{mh(x)+(x-\alpha)h'(x)}$, $x_{k+1}=x_k-\frac{f(x_k)f'(x_k)}{[f'(x_k)]^2-f(x_k)f''(x_k)}$

简化牛顿法： $x_{k+1}=x_k-Cf(x_k),C=\frac{1}{f'(x_0)}$

下山法： $x_{k+1}=\lambda x_{k+1}+(1-\lambda)x_k$, $x_{k+1}=x_k-\lambda\frac{f(x_k)}{f'(x_k)},k=$

$0,1,2,\cdots$, 从 $\lambda=1$ 开始逐次将 λ 折半直到 $|f(x_{k+1})|<|f(x_k)|$

割线法：单点弦截: $x_{k+1}=x_k-\frac{f(x_k)}{f(x_k)-f(x_0)}(x_k-x_0)$

两点弦截法: $x_{k+1}=x_k-\frac{f(x_k)}{f(x_k)-f(x_{k-1})}(x_k-x_{k-1})$

解非线性方程组： $x^{k+1}=x^k-(f'(x^k))^{-1}f(x^k)$

$$f'(x)=\begin{bmatrix}\frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n}\\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n}\\ \vdots & \vdots & \ddots & \vdots\\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n}\end{bmatrix}$$

09 常微分方程初值问题的数值解法

一阶常微分方程初值问题 $\begin{cases}y'=\frac{dy}{dx}=f(x,y),\ \ x\in[x_0,b]\\ y(x_0)=y_0\end{cases}$

Lipschitz: $\forall x_0\in[a,b],y_0\in R,|f(x,y)-f(x,\bar{y})|\leq L|y-\bar{y}|$

则常微分方程初值问题存在唯一的连续可微解 y(x)

前向欧拉法： $\frac{y_{n+1}-y_n}{x_{n+1}-x_n}=f(x_n,y_n)$， $y_{n+1}=y_n+hf(x_n,y_n)$

$$y(x_{n+1})=y(x_n+h)=y(x_n)+\boldsymbol{y'(x_n)}h+\frac{h^2}{2}y''(\xi_n)$$

$$y_n=y(x_n),\ f(x_n,y_n)=f(x_n,y(x_n))=\boldsymbol{y'(x_n)}$$

$$y(x_{n+1})-y_{n+1}=\frac{h^2}{2}y''(\xi_n)\ \approx\frac{h^2}{2}y''(x_n)$$

后向欧拉法（隐式,一阶）： $y_{n+1}=y_n+hf(x_{n+1},y_{n+1})$

$y_{n+1}^{(0)}=y_n+hf(x_n,y_n)$, $y_{n+1}^{(k+1)}=y_n+hf(x_{n+1},y_{n+1}^{(k)})$ $k=1,2\ldots$ (迭代法)

$|y_{n+1}^{(k+1)}-y_{n+1}|=h|f(x_{n+1},y_{n+1}^{(k)})-f(x_{n+1},y_{n+1})|\leq$
$hL|y_{n+1}^{(k)}-y_{n+1}|\leq\cdots\leq(hL)^{k+1}|y_{n+1}^{(0)}-y_{n+1}|$ hL<1 收敛

梯形方法（隐式,二阶）： $y_{n+1}=y_n+\frac{h}{2}[f(x_n,y_n)+$

$f(x_{n+1},y_{n+1})]$ $y_{n+1}^{(0)}=y_n+hf(x_n,y_n)$ $y_{n+1}^{(k+1)}=y_n+$

$\frac{h}{2}[f(x_n,y_n)+f(x_{n+1},y_{n+1}^{(k)})]$ $(k=1,2,\cdots)$ (迭代法)

$y_{n+1}-y_{n+1}^{(k+1)}=\frac{h}{2}\left[f(x_{n+1},y_{n+1})-f(x_{n+1},y_{n+1}^{(k)})\right]\leq$

$\frac{hL}{2}\left|y_{n+1}-y_{n+1}^{(k)}\right|\leq\cdots\leq\left(\frac{hL}{2}\right)^{k+1}\left|y_{n+1}-y_{n+1}^{(0)}\right|$

改进欧拉法/Heun 法：

预测： $\overline{y_{n+1}}=y_n+hf(x_n,y_n)$

校正： $y_{n+1}=y_n+\frac{h}{2}[f(x_n,y_n)+f(x_{n+1},\overline{y_{n+1}})]$

$$\begin{cases}y_p=y_n+hf(x_n,y_n)\\ y_c=y_n+hf(x_{n+1},y_p)\\ y_{n+1}=(y_p+y_c)/2\end{cases}$$

显式单步法的**局部截断误差**： $y_{n+1}=y_n+h\phi(x_n,y_n,h)$

$$T_{n+1}=y(x_{n+1})-y(x_n)-h\phi(x_n,y(x_n),h)$$

p 阶精度： $T_{n+1}=y(x+h)-y(x)-h\phi(x,y,h)=O(h^{p+1})$

$y(x_{n+1})=y(x_n)+y'(x_n)h+\frac{y''(x_n)}{2!}h^2+\cdots+$

$\frac{y^{(p)}(x_n)}{p!}h^p+\frac{y^{(p+1)}(\xi)}{(p+1)!}h^{p+1}$

二阶显式 R-K 方法: $c_2\lambda_2=\frac{1}{2},c_2\mu_{21}=\frac{1}{2},c_1+c_2=1$

$$\begin{cases}y_{n+1}=y_n+h(c_1K_1+c_2K_2)\\ K_1=f(x_n,y_n)\\ K_2=f(x_n+\lambda_2h,y_n+\mu_{21}hK_1)\end{cases}$$

令 $c_2=a\neq 0$,则 $c_1=1-a,\lambda_2=\mu_{21}=\frac{1}{2a}$

中点公式： $a=1,\ c_2=1,\ c_1=0,\ \lambda_2=\mu_{21}=\frac{1}{2}$

$$\begin{cases} y_{n+1} = y_n + hk_2 \\ K_1 = f(x_n, y_n) \\ K_2 = f(x_n + h/2, y_n + hK_1/2) \end{cases}$$ 也可写为

$$y_{n+1} = y_n + hf\left(x_n + \frac{h}{2}, y_n + \frac{h}{2} f(x_n, y_n)\right)$$

三阶龙格-库塔（库塔格式）$O(h^3)$：

$$\begin{cases} y_{i+1} = y_i + \frac{h}{6}(K_1 + 4K_2 + K_3) \\ K_1 = f(x_i, y_i) \\ K_2 = f(x_i + \frac{h}{2}, y_i + \frac{h}{2} K_1) \\ K_3 = f(x_i + h, y_i - hK_1 + 2hK_2) \end{cases}$$

四阶显式 R-K 方法 $O(h^4)$：

$$y_{n+1} = y_n + \frac{h}{6}(K_1 + 2K_2 + 2K_3 + K_4)$$

$K_1 = f(x_n, y_n)$ $K_2 = f(x_n + \frac{h}{2}, y_n + \frac{h}{2} K_1)$

$K_3 = f(x_n + \frac{h}{2}, y_n + \frac{h}{2} K_2)$ $K_4 = f(x_n + h, y_n + hK_3)$

单步法的收敛性：假设单步法具有 p 阶精度，且增量函数满足利普西茨条件 $|\phi(x, y, h) - \phi(x, \bar{y}, h)| \le L_\phi |y - \bar{y}|$；如果 $y_0 = y(x_0)$ 则整体截断误差$|y(x_n) - y_n| = O(h^p)$, $1 + hL \le e^{hL}$, $(1 + hL)^n \le e^{nhL} \le e^{L(b-a)}$

单步法的稳定性：$y' = \lambda y = f(x, y), \lambda$ 是复数且 $\mathrm{real}(\lambda) < 0$

当方法稳定时要求变量 λh 的取值范围称为方法的绝对稳定域，它与实轴的交集称为绝对稳定区间. 即迭代系数绝对值小于 1

$y_{n+1} = y_n + \frac{h}{2}\lambda(y_n + y_{n+1})$, $y_{n+1} = \frac{1 + \frac{1}{2}\lambda h}{1 - \frac{1}{2}\lambda h} y_n$, $\left|\frac{1 + \frac{1}{2}\lambda h}{1 - \frac{1}{2}\lambda h}\right| < 1$

Euler 方法(1), (-2,0)；梯形法(2), $(-\infty, 0)$；Heun 法(2), (-2,0)

二阶 R-K(2), (-2,0)；三阶 R-K(3), (-2.51, 0)；四阶 R-K(4), (-2.78, 0)

1）收敛性是反映差分公式本身的**截断误差**对数值解的影响；

2）稳定性是反映计算过程中**舍入误差**对数值解的影响；

3）只有即收敛又稳定的差分公式才有实用价值；

线性多步法：r+1 步线性多步方法, $\beta_{-1} \ne 0$ 时为隐式公式

$$y_{n+1} = \sum_{i=0}^{r} \alpha_i y_{n-i} + h \sum_{\boldsymbol{i=-1}}^{r} \beta_i f_{n-i}$$

r+1 步 Adams 显式公式：$y_{n+1} = y_n + h\sum_{j=0}^{r} \beta_{rj} f_{n-j}$

$r = 0, p = 1$ $y_{n+1} = y_n + hf_n + (1/2)h^2 y''(x_n)$

$r = 1, p = 2$ $y_{n+1} = y_n + (h/2)(3f_n - f_{n-1}) + (5/12)h^3 y'''(x_n)$

$r = 2, p = 3$ $y_{n+1} = y_n + (h/12)(23f_n - 16f_{n-1} + 5f_{n-2}) + (3/8)h^4 y^{(4)}(x_n)$

$r = 3, p = 4$ $y_{n+1} = y_n + (h/24)(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3}) + (251/720)h^5 y^{(5)}(x_n)$

Adams 隐式公式：$y_{n+1} = y_n + h\sum_{\boldsymbol{j=0}}^{r} \beta_{rj}^* f_{n-j+1}$

$r = 0, p = 1$ $y_{n+1} = y_n + hf_{n+1} - (1/2)h^2 y''(x_n)$

$r = 1, p = 2$ $y_{n+1} = y_n + (h/2)(f_n + f_{n+1}) - (1/12)h^3 y''(x_n)$

$r = 2, p = 3$ $y_{n+1} = y_n + (h/12)(5f_{n+1} + 8f_n - f_{n-1}) - (1/24)h^4 y^{(4)}(x_n)$

$r = 3, p = 4$ $y_{n+1} = y_n + (h/24)(9f_{n+1} + 19f_n - 5f_{n-1} + f_{n-2}) - (19/720)h^5 y^{(5)}(x_n)$

四阶 Adams 预估-校正公式：$\bar{f}_{n+1} = f(x_{n+1}, \bar{y}_{n+1})$

预测：$\bar{y}_{n+1} = y_n + (h/24)(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3})$

校正：$y_{n+1} = y_n + (h/24)(9\bar{f}_{n+1} + 19f_n - 5f_{n-1} + f_{n-2})$

用 4 阶 R-K 公式启动，即提供初始值 y_1, y_2, y_3，注意 y_0已知

米尔尼方法：$y_{n+4} = y_n + \frac{4h}{3}(2f_{n+3} - f_{n+2} + 2f_{n+1}) + \frac{14}{45}h^5 y^{(5)}(x_n) + O(h^6)$

一阶 ODE 方程组：预测：$\overline{y_{i+1}} = y_i + hf(x_i, y_i, z_i)$

$\overline{z_{i+1}} = z_i + hg(x_i, y_i, z_i)$ （Heun 法）

校正：$y_{i+1} = y_i + \frac{h}{2}[f(x_i, y_i, z_i) + f(x_{i+1}, \overline{y_{i+1}}, \overline{z_{i+1}})]$

$z_{i+1} = z_i + \frac{h}{2}[g(x_i, y_i, z_i) + g(x_{i+1}, \overline{y_{i+1}}, \overline{z_{i+1}})]$

R-K 方法解方程组：

$y_{i+1} = y_i + \frac{h}{6}[K_1 + 2K_2 + 2K_3 + K_4]$

$z_{i+1} = z_i + \frac{h}{6}[L_1 + 2L_2 + 2L_3 + L_4]$

$K_1 = f(x_i, y_i, z_i)$ $L_1 = g(x_i, y_i, z_i)$

$K_2 = f\left(x_i + \frac{h}{2}, y_i + \frac{h}{2}K_1, z_i + \frac{h}{2}L_1\right)$ $L_2 = g\left(x_i + \frac{h}{2}, y_i + \frac{h}{2}K_1, z_i + \frac{h}{2}L_1\right)$ $K_3 = f\left(x_i + \frac{h}{2}, y_i + \frac{h}{2}K_2, z_i + \frac{h}{2}L_2\right)$

$L_3 = g\left(x_i + \frac{h}{2}, y_i + \frac{h}{2}K_2, z_i + \frac{h}{2}L_2\right)$ $K_4 = f(x_i + h, y_i + hK_3, z_i + hL_3)$ $L_4 = g(x_i + h, y_i + hK_3, z_i + hL_3)$

高阶方程：$\frac{d^m y}{dx^m} = f_1(x, y, y', \cdots, y^{(m-1)})$； $a \le x \le b$

$y(a) = \eta_1, y'(a) = \eta_2, y^{(m-1)}(a) = \eta_m$

令 $y = y_1$, $\frac{dy_1}{dx} = y_2$, $\frac{dy_{m-1}}{dx} = y_m$ 则有 $\frac{dy_1}{dx} = y_2 \dots \frac{dy_m}{dx} = f(x, y_1, \dots, y_m)$； $y_1(a) = \eta_1 \dots y_m(a) = \eta_m$ 令 $y_1 = y$, $y_2 = y'$

Taylor: $f(x + h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \cdots + \frac{h^n}{n!}f^{(n)}(x) + R_n(x, h)$, $R_n(x, h) = \frac{h^{n+1}}{(n+1)!}f^{(n+1)}(c)$

$f(x_n + \lambda_2 h, y_n + \mu_{21}hf_n) = f_n + f_x'(x_n, y_n)\lambda_2 h + f_y'(x_n, y_n)\mu_{21}hf_n + 1/2! * [f_x''(x_n, y_n)(\lambda_2 h)^2 + f_{xy}''(x_n, y_n)(\lambda_2 h)(\mu_{21}hf_n) + f_y''(x_n, y_n)(\mu_{21}hf_n)^2] + O(h^3)$

$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \ldots + \frac{x^n}{n!} + \ldots = \sum_{n=0}^{\infty} \frac{x^n}{n!}$

$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \frac{x^9}{9!} - \ldots + (-1)^n \frac{x^{2n+1}}{(2n+1)!} + \ldots = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n+1}}{(2n+1)!}$

$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \frac{x^8}{8!} - \ldots + (-1)^n \frac{x^{2n}}{(2n)!} + \ldots = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n}}{(2n)!}$

$\arctan x = x - \frac{x^3}{3} + \frac{x^5}{5} - \cdots + \frac{(-1)^n x^{2n+1}}{2n+1} + \cdots = \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+1}}{2n+1}$

$\ln(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \cdots + \frac{(-1)^n x^{n+1}}{n+1} + \cdots = \sum_{n=0}^{\infty} (-1)^n \frac{x^{n+1}}{n+1}$

$(1 + x)^\alpha = 1 + \alpha x + \frac{\alpha(\alpha-1)}{2!}x^2 + \cdots + \frac{\alpha(\alpha-1)\ldots(\alpha-n+1)}{n!}x^n + \ldots = 1 + \sum_{n=1}^{\infty} \frac{\alpha(\alpha-1)\cdots(\alpha-n+1)}{n!}x^n$