计算方法

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第四章多项式插值与函数最佳逼近

本章主要内容

1. Lagrange插值多项式及余项表示
2. 差商和Newton插值多项式
3. Hermite插值多项式
4. 高次插值的缺点及分段插值
5. 三次样条插值
6. 最佳一致逼近
7. 最佳平方逼近

为什么要用插值或函数逼近?

1. 函数关系$y = f(x)$是一个函数表: $y_i = f(x_i)$ $(i = 0, 1, 2 \cdots, n)$;
2. 函数解析表达式$y = f(x)$知道, 但很复杂.

用一个简单的函数(一般是多项式)$P(x)$近似函数$f(x)$.

什么是插值?

定义4.1

设函数$y=f(x)$在区间$[a,b]$上有定义, 且已知在点$a\leq x_0<x_1<\cdots<x_n\leq b$上的值$y_0,y_1,\cdots,y_n$, 若存在一个简单函数$P(x)$, 使

$$P(x_i)=y_i \quad (i=0,1,2\cdots,n) \tag{1}$$

成立,则称$P(x)$为$f(x)$的插值函数, 点$x_0,x_1,\cdots,x_n$称为插值节点, $[a,b]$称为插值区间, 求$P(x)$的方法称为插值法. 若$P(x)$ 是次数不超过n的多项式, 即

$$P(x)=a_0+a_1x+\cdots+a_nx^n, \tag{2}$$

则称$P(x)$为插值多项式.

在几何上, 插值法就是求曲线$y=P(x)$, 使其通过给定的$n+1$个点(x_i,y_i), $i=0,1,\cdots,n$.

定理4.1

满足插值条件*(1)*的n次多项式是存在唯一的。

4.1 拉格朗日(Lagrange)插值

问题 求n次多项式$l_k(x)$，使满足

$$l_k(x_0)=0,\ l_k(x_1)=0,\ \cdots,\ l_k(x_{k-1})=0,\ l_k(x_k)=1,$$
$$l_k(x_{k+1})=0,\cdots,\ l_k(x_n)=0.$$

即

$$l_k(x_j)=\begin{cases}1 & (j=k)\\ 0 & (j\neq k).\end{cases} \tag{3}$$

由条件(3)知道$x_0,\ x_1,\ \cdots,\ x_{k-1},\ x_{k+1},\ \cdots,\ x_n$ 是n 次多项式$l_k(x)$的零点，所以$l_k(x)$ 有n 个因子：

$$x-x_0,\ x-x_1,\ \cdots,\ x-x_{k-1},\ x-x_{k+1},\cdots,\ x-x_n.$$

所以有

$$\begin{aligned} l_k(x) &= A_k(x-x_0)(x-x_1)\cdots(x-x_{k-1})(x-x_{k+1})\cdots(x-x_n)\\ &= A_k\prod_{\substack{i=0\\ i\neq k}}^{n}(x-x_i) \end{aligned} \tag{4}$$

其中A_k为待定常数. 由$l_k(x_k)=1$, 即

$$A_k\prod_{\substack{i=0\\i\neq k}}^{n}(x_k-x_i)=1$$

得到

$$A_k=\frac{1}{\prod\limits_{\substack{i=0\\i\neq k}}^{n}(x_k-x_i)}\quad\Rightarrow$$

$$l_k(x)=\frac{1}{\prod\limits_{\substack{i=0\\i\neq k}}^{n}(x_k-x_i)}\cdot\prod_{\substack{i=0\\i\neq k}}^{n}(x-x_i)=\frac{\prod\limits_{\substack{i=0\\i\neq k}}^{n}(x-x_i)}{\prod\limits_{\substack{i=0\\i\neq k}}^{n}(x_k-x_i)}=\prod_{\substack{i=0\\i\neq k}}^{n}\frac{x-x_i}{x_k-x_i}.\quad(5)$$

$l_k(x)$称为n次基本插值多项式. 当$k=0,1,\cdots,n$时, 可得到$n+1$个基本插值多项式$l_0(x),l_1(x),\cdots,l_n(x)$.

Lagrange插值多项式

利用基本插值多项式，满足插值条件(1)的n次插值多项式可以表示为

$$P(x) = \sum_{k=0}^{n} f(x_k) l_k(x). \tag{6}$$

事实上，由于$P(x)$是n次多项式，而且

$$P(x_i) = \sum_{k=0}^{n} f(x_k) l_k(x_i) = f(x_i) l_i(x_i) = f(x_i), \quad (i = 0, 1, \cdots, n.)$$

(6)称为n次Lagrange 插值多项式，记为$L_n(x)$，即

$$L_n(x) = \sum_{k=0}^{n} f(x_k) l_k(x) = \sum_{k=0}^{n} f(x_k) \prod_{\substack{i=0 \\ i \neq k}}^{n} \frac{x - x_i}{x_k - x_i} \tag{7}$$

注1

$l_0(x), l_1(x) \cdots, l_n(x)$线性无关，它是$n$次多项式空间$\mathcal{P}_n$的一组基，而 $1, x, x^2, \cdots, x^n$也是其一组基. $l_0(x), l_1(x) \cdots, l_n(x)$称为$n$次*Lagrange* 插值基函数.

定理4.2

设$x_0, x_1, \cdots, x_n$是互异节点，则存在唯一的次数不超过n次的多项式$L_n(x)$，使得

$$L_n(x_i) = f(x_i), \quad (i = 0, 1, \cdots, n)$$

证　存在性已得．现唯一性．假设另有n次多项式$q_n(x)$满足插值条件(1)，即

$$q_n(x_i) = f(x_i), \quad (i = 0, 1, 2 \cdots, n.)$$

令$h(x) = L_n(x) - q_n(x)$，则有

$$h(x_i) = 0, \quad (i = 0, 1, 2 \cdots, n.)$$

即$h(x)$有$n+1$个不同零点，$\Longrightarrow h(x) \equiv 0.$

称$R_n(x)=f(x)-L_n(x)$为插值多项式的余项.

定理4.3

设$f^{(n)}(x)$ 在$[a,b]$ 上连续, $f^{(n+1)}(x)$ 在(a,b) 内存在, $x_0, x_1, \cdots,$ $x_n \in [a,b]$ 为互异节点, $L_n(x)$ 是满足*(1)*的插值多项式, 则对$\forall x \in [a,b]$, $\exists\, \xi \in (a,b)$ (ξ 依赖于x), 使得

$$R_n(x)=f(x)-L_n(x)=\frac{f^{(n+1)}(\xi)}{(n+1)!}\omega_{n+1}(x), \tag{8}$$

其中$\omega_{n+1}(x)=\prod_{i=0}^{n}(x-x_i)$.

注2

1. ξ依赖于x，即

$$\xi=\xi(x)\in(\min\{x_0,x_1,\cdots,x_n\},\max\{x_0,x_1,\cdots,x_n\}).$$

2. 当$f(x)$本身是一个次数不超过n的多项式时，
$f(x)-L_n(x)=0$，因而$L_n(x)=f(x)$. 特别当$f(x)=1$，则有

$$\sum_{k=0}^{n} l_k(x)=1$$

3. 由于ξ一般不能精确求出，因此只能估计误差.
设$\max\limits_{a\le x\le b}|f^{(n+1)}(x)|=M_{n+1}$，则有

$$|R_n(x)|\le\frac{M_{n+1}}{(n+1)!}|\omega(x)|$$

例4.1

给定$\sin 0.32 = 0.314567$, $\sin 0.34 = 0.333487$, $\sin 0.36 = 0.352274$, 用线性(1次)及抛物(2次)插值计算$\sin 0.3367$的值并估计误差.

解 令$x_0 = 0.32$, $x_1 = 0.34$, $x_2 = 0.36$, $y_0 = 0.314567$, $y_1 = 0.333487$, $y_2 = 0.352274$.

(1) 用线性插值.

$$L_1(x) = y_0 \frac{x - x_1}{x_0 - x_1} + y_1 \frac{x - x_0}{x_1 - x_0},$$

$$\sin 0.3367 \approx L_1(0.3367) = 0.330365,$$

$$|R_1(x)| \leq \frac{M_2}{2} |(x - x_0)(x - x_1)|,$$

其中$M_2 = \max\limits_{x_0 \leq x \leq x_1} |f''(x)| = \max\limits_{x_0 \leq x \leq x_1} |\sin x| \leq \sin x_1 = 0.3335$,

所以

$$|R_1(0.3367)| \leq \frac{1}{2} \times 0.3335 \times 0.0167 \times 0.0033 = 0.92 \times 10^{-5}.$$

(2) 用抛物插值.

$$L_2(x) = y_0\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + y_1\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + y_2\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}$$

$$\sin 0.3367 \approx L_2(0.3367) = 0.330374.$$

$$|R_2(x)| \le \frac{M_3}{3!}|(x-x_0)(x-x_1)(x-x_2)|,$$

其中 $M_2 = \max\limits_{x_0\le x\le x_2} |f^{(3)}(x)| = \max\limits_{x_0\le x\le x_2} |\cos x_0| = 0.828$, 所以

$$|R_2(0.3367)| \le \frac{1}{6}\times 0.838\times 0.0167\times 0.033\times 0.0233 = 0.178\times 10^{-6}.$$

例4.2

在工程中的一个函数

$$f(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

的函数值已造成函数表. 假设在区间[4, 6]上用线性插值计算$f(x)$的近似值, 问会有多大的误差?

解 在[4,6]上作$f(x)$的线性插值多项式$p_1(x)$, 则

$$R_1(x) = f(x) - p_1(x) = \frac{1}{2} f''(\xi)(x - x_0)(x - x_1), \quad \xi \in [4, 6],$$

$$f'(x) = \frac{2}{\sqrt{\pi}} e^{-x^2}, \quad f''(x) = -\frac{4x}{\sqrt{\pi}} e^{-x^2},$$

$$f'''(x) = \frac{4}{\sqrt{\pi}} (2x^2 - 1) e^{-x^2} > 0, \quad x \in (4, 6), \Longrightarrow f''(x) \nearrow$$

所以有

$$|R_2(x)| \le \frac{1}{2} \times |f''(4)| \times |(5-4)(5-6)| = 0.508 \times 10^{-6}.$$

4.2 差商、差分与牛顿插值

Lagrange插值的缺点：当节点增加或减少时，插值多项式$L_n(x)$ 将发生变化，计算不便.

设$L_{k-1}(x)$是以$x_0, x_1, \cdots, x_{k-1}$ 为插值节点的$f(x)$ 的$k-1$ 次插值多项式，$L_k(x)$是以$x_0, x_1, \cdots, x_{k-1}, x_k$ 为插值节点的$f(x)$ 的k 次插值多项式,考察L_{k-1} 和$L_k(x)$ 之间的关系. 令

$$g(x) = L_k(x) - L_{k-1}(x),$$

则$g(x)$是次数不超过k的多项式，且对$j = 0, 1, \cdots, k-1$有

$$\begin{aligned} g(x_j) &= L_k(x_j) - L_{k-1}(x_j) = f(x_j) - f(x_j) = 0. \quad \Longrightarrow \\ g(x) &= a_k(x - x_0)(x - x_1)\cdots(x - x_{k-1}) \end{aligned}$$

其中a_k是和x无关的常数. 也可以写成

$$\begin{aligned} L_k(x) &= L_{k-1}(x) + a_k(x - x_0)(x - x_1)\cdots(x - x_{k-1}), \quad (9) \\ L_k(x) &= a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \cdots \\ &\quad + a_k(x - x_0)(x - x_1)\cdots(x - x_{k-1}). \end{aligned}$$

下面求a_k, 在(9)中令$x = x_k$得

$$
\begin{aligned}
a_k &= \frac{L_k(x_k) - L_{k-1}(x_k)}{(x_k - x_0)(x_k - x_1)\cdots(x_k - x_{k-1})} \\
&= \frac{f(x_k) - \sum\limits_{m=0}^{k-1} f(x_m) \prod\limits_{\substack{i=0 \\ i \neq m}}^{k-1} \frac{x_k - x_i}{x_m - x_i}}{\prod\limits_{i=0}^{k-1} (x_k - x_i)} \\
&= \frac{f(x_k)}{\prod\limits_{i=0}^{k-1} (x_k - x_i)} - \sum_{m=0}^{k-1} \frac{f(x_m)}{(x_k - x_m) \prod\limits_{\substack{i=0 \\ i \neq m}}^{k-1} (x_m - x_i)} \\
&= \sum_{m=0}^{k} \frac{f(x_m)}{\prod\limits_{\substack{i=0 \\ i \neq m}}^{k} (x_m - x_i)} \qquad (10)
\end{aligned}
$$

定义4.2

设已知函数$f(x)$ 在$n+1$ 个互异节点$x_0, x_1, \cdots, x_n$ 上的函数值为$f(x_0)$, $f(x_1)$, $\cdots$, $f(x_n)$, 称

$$f[x_i, x_j] = \frac{f(x_j) - f(x_i)}{x_j - x_i}$$

为$f(x)$ 关于节点x_i, x_j 的*1*阶差商*(*均差*)*. 称*1*阶差商$f[x_i, x_j]$ 和 $f[x_j, x_k]$ 的差商

$$f[x_i, x_j, x_k] = \frac{f[x_j, x_k] - f[x_i, x_j]}{x_k - x_i}$$

为$f(x)$ 关于节点x_i, x_j, x_k 的*2*阶差商, 一般地, 称*2*个$k-1$ 阶的差商为k 阶差商, 即

$$\begin{aligned} & f[x_0, x_1, \cdots, x_{k-1}, x_k] \\ = & \frac{f[x_1, x_2, \cdots, x_{k-1}, x_k] - f[x_0, x_1, \cdots, x_{k-2}, x_{k-1}]}{x_k - x_0}. \end{aligned}$$

约定*0*阶差商是函数值.

计算函数的差商，可以通过列表法计算。

i	x_i	$f(x_i)$	$f[x_i, x_{i+1}]$	$f[x_i, x_{i+1}, x_{i+2}]$	$f[x_i, x_{i+1}, x_{i+2}, x_{i+3}]$
0	x_0	$f(x_0)$	$f[x_0, x_1]$	$f[x_0, x_1, x_2]$	$f[x_0, x_1, x_2, x_3]$
1	x_1	$f(x_1)$	$f[x_1, x_2]$	$f[x_1, x_2, x_3]$	
2	x_2	$f(x_2)$	$f[x_2, x_3]$		
3	x_3	$f(x_3)$			

差商有下列性质：

性质1

k阶差商可表示成函数值$f(x_0), f(x_1), \cdots, f(x_k)$的线性组合，即

$$f[x_0, x_1, \cdots, x_k] = \sum_{m=0}^{k} \frac{f(x_m)}{\prod\limits_{\substack{i=0 \\ i\neq m}}^{k} (x_m - x_i)}. \tag{11}$$

证 用归纳法. 当$k=0$时结论显然成立. 设$k=l-1$时结论成立, 即有

$$f[x_0,x_1,\cdots,x_{l-1}] = \sum_{m=0}^{l-1}\frac{f(x_m)}{\prod\limits_{\substack{i=0\\i\neq m}}^{l-1}(x_m-x_i)},$$

$$f[x_1,x_2,\cdots,x_l] = \sum_{m=1}^{l}\frac{f(x_m)}{\prod\limits_{\substack{i=1\\i\neq m}}^{l}(x_m-x_i)}.$$

于是$f[x_0, x_1, x_2, \cdots, x_l]$

$$= \frac{1}{x_l - x_0}(f[x_1, x_2, \cdots, x_l] - f[x_0, x_1, \cdots, x_{l-1}])$$

$$= \frac{1}{x_l - x_0}\left\{\sum_{m=1}^{l} \frac{f(x_m)}{\prod\limits_{\substack{i=1\\ i\neq m}}^{l}(x_m - x_i)} - \sum_{m=0}^{l-1} \frac{f(x_m)}{\prod\limits_{\substack{i=0\\ i\neq m}}^{l-1}(x_m - x_i)}\right\}$$

$$= \frac{1}{x_0 - x_l}\frac{f(x_0)}{\prod\limits_{i=1}^{l-1}(x_0 - x_i)} + \frac{1}{x_l - x_0}\sum_{m=1}^{l-1}\left(\frac{f(x_m)}{\prod\limits_{\substack{i=1\\ i\neq m}}^{l}(x_m - x_i)} - \frac{f(x_m)}{\prod\limits_{\substack{i=0\\ i\neq m}}^{l-1}(x_m - x_i)}\right)$$

$$+\frac{1}{x_l - x_0}\frac{f(x_l)}{\prod\limits_{i=1}^{l-1}(x_l - x_i)} = \sum_{m=0}^{l} \frac{f(x_m)}{\prod\limits_{\substack{i=0\\ i\neq m}}^{l}(x_m - x_i)}.$$

性质2

k阶差商$f[x_0, x_1, \cdots, x_k]$与节点的次序无关. 即

$$f[x_0, \cdots, x_i, \cdots, x_j, \cdots, x_k] = f[x_0, \cdots, x_j, \cdots, x_i, \cdots, x_k], \quad 0 \le i, j \le k.$$

性质3

k阶差商和k阶导数之间有如下关系：

$$f[x_0, x_1, \cdots, x_k] = \frac{f^{(k)}(\eta)}{k!}, \tag{12}$$

其中$\eta \in (\min\{x_0, x_1, \cdots, x_k\}, \max\{x_0, x_1, \cdots, x_k\})$.

由(10)和(11)知, $a_k = f[x_0, x_1, \cdots, x_k]$. 利用(9)可得

$$\begin{aligned} L_n(x) &= f(x_0) + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) \\ &+ \cdots + f[x_0, x_1, \cdots, x_n](x - x_0)(x - x_1) \cdots (x - x_{n-1}). \end{aligned} \tag{13}$$

(13)式右端称为n次Newton插值多项式.

证 以$x_0,x_1,\cdots,x_k$为节点作$f(x)$的k次Newton插值

$$\begin{aligned}N_k(x) &= f(x_0)+f[x_0,x_1](x-x_0)+f[x_0,x_1,x_2](x-x_0)(x-x_1)\\ &\quad +\cdots+f[x_0,x_1,\cdots,x_k](x-x_0)(x-x_1)\cdots(x-x_{k-1}),\end{aligned}$$

考察余项

$$R_k(x)=f(x)-N_k(x),$$

易知对$i=0,1,\cdots,k$有$R(x_i)=0$, 即$R_k(x)$有$k+1$个互异的零点.由Rolle定理知相邻2个零点之间至少有$R_k'(x)$的1个零点, 从而$R_k'(x)$至少有k个不同零点. 依次类推, $R_k^{(k)}(x)$至少有一个零点, 记为η, 即有

$$R_k^{(k)}(\eta)=f^{(k)}(\eta)-N_k^{(k)}(\eta)=f^{(k)}(\eta)-k!f[x_0,x_1,\cdots,x_k]=0,$$

因此

$$f[x_0,x_1,\cdots,x_k]=\frac{f^{(k)}(\eta)}{k!}.$$

利用差商定义及性质2可得Newton插值的余项.

$$
\begin{aligned}
&f(x) = f(x_0) + f[x, x_0](x - x_0),\\
&f[x, x_0] = f[x_0, x_1] + f[x, x_0, x_1](x - x_1),\\
&\dots\\
&f[x, x_0, \cdots, x_{n-1}] = f[x_0, x_1, \cdots, x_n] + f[x, x_0, \cdots, x_n](x - x_n).
\end{aligned}
$$

将后一项代入前易项, 得

$$
\begin{aligned}
f(x) &= f(x_0) + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1)\\
&\quad + \cdots + f[x_0, x_1, \cdots, x_n](x - x_0)(x - x_1)\cdots(x - x_{n-1})\\
&\quad + f[x, x_0, \cdots, x_n](x - x_0)(x - x_1)\cdots(x - x_n)\\
&= N_n(x) + R_n(x).
\end{aligned}
$$

所以Newton插值余项为

$$
R_n(x) = f[x, x_0, \cdots, x_n]\omega_{n+1}(x).
$$

4.3 差分及等距节点插值

等距节点的Newton插值, 此时差商可以更简单地表示, 即差分.
设函数$y = f(x)$在等距节点$x_k = x_0 + kh(k = 0, 1, \cdots, n)$上的函数值为$f_i = f(x_k)$, 这里$h$为常数, 称步长.

定义4.3

记号

$$\triangle f_k = f_{k+1} - f_k, \tag{14}$$

$$\nabla f_k = f_k - f_{k-1}, \tag{15}$$

$$\delta f_k = f_{k+1/2} - f_{k-1/2} \tag{16}$$

分别称为$f(x)$在x_k处以步长h的一阶向前差分, 向后差分及中心差分. 二阶差分可定义为

$$\begin{aligned}
\triangle^2 f_k &= \triangle f_{k+1} - \triangle f_k \\
\nabla^2 f_k &= \nabla f_k - \nabla f_{k-1} \\
\delta^2 f_k &= \delta f_{k+1/2} - \delta f_{k-1/2}.
\end{aligned}$$

一般地可定义m阶差分为

$$
\begin{aligned}
\triangle^m f_k &= \triangle^{m-1} f_{k+1} - \triangle^{m-1} f_k \\
\nabla^m f_k &= \nabla^{m-1} f_k - \nabla^{m-1} f_{k-1} \\
\delta^m f_k &= \delta^{m-1} f_{k+1/2} - \delta^{m-1} f_{k-1/2}.
\end{aligned}
$$

算子$\triangle, \nabla, \delta$称为向前差分算子, 向后差分算子及中心差分算子, 记I为恒等算子, E为移位算子, 定义为

$$
If_k = f_k, \quad Ef_k = f_{k+1},
$$

于是可得

$$
\triangle = E - I, \quad \nabla = I - E^{-1}, \quad \delta = E^{1/2} - E^{-1/2}.
$$

性质4

各阶差分都可以用函数值表示.

$$\begin{aligned}\triangle^n f_k &= (E-I)^n f_k = \sum_{j=0}^{n}(-1)^j C_n^j E^{n-j} f_k \\ &= \sum_{j=0}^{n}(-1)^j C_n^j f_{n+k-j} \end{aligned} \tag{17}$$

$$\begin{aligned}\nabla^n f_k &= (I-E^{-1})^n f_k = \sum_{j=0}^{n}(-1)^{n-j} C_n^j E^{j-n} f_k \\ &= \sum_{j=0}^{n}(-1)^{n-j} C_n^j f_{k+j-n}. \end{aligned} \tag{18}$$

性质5

可用各阶差分表示函数值.

$$f_{n+k} = E^n f_k = (I + \triangle)^n f_k = \sum_{j=0}^{n} C_n^j \triangle^j f_k. \tag{19}$$

性质6

差商和差分有如下关系：

$$f[x_k, x_{k+1}, \cdots, x_{k+m}] = \frac{1}{m!}\frac{1}{h^m}\triangle^m f_k, \quad (m = 1, 2, \cdots, n). \tag{20}$$

$$f[x_k, x_{k-1}, \cdots, x_{k-m}] = \frac{1}{m!}\frac{1}{h^m}\nabla^m f_k, \quad (m = 1, 2, \cdots, n). \tag{21}$$

利用(12)和(20)可得

$$\triangle^n f_k = h^n f^{(n)}(\xi), \quad \xi \in (x_k, x_k + n). \tag{22}$$

差分的计算也可以列表计算.

f_k	$\triangle$	$\triangle^2$	$\triangle^3$	$\triangle^4$	$\cdots$
f_0	$\triangle f_0$	$\triangle^2 f_0$	$\triangle^3 f_0$	$\triangle^4 f_0$	$\vdots$
f_1	$\triangle f_1$	$\triangle^2 f_1$	$\triangle^3 f_1$	$\vdots$	
f_2	$\triangle f_2$	$\triangle^2 f_2$	$\vdots$		
f_3	$\triangle f_3$	$\vdots$			
f_4	$\vdots$				
$\vdots$					

f_k	∇	∇^2	∇^3	∇^4	$\cdots$	
f_0						
f_1	∇f_1					
f_2	∇f_2	$\nabla^2 f_2$				
f_3	∇f_3	$\nabla^2 f_3$	$\nabla^3 f_3$			
f_4	∇f_4	$\nabla^2 f_4$	$\nabla^3 f_4$	$\nabla^4 f_4$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\cdots$

设$x = x_0 + th$, $0 \le t \le 1$, 则

$$\omega_{k+1}(x) = \prod_{j=0}^{k}(x - x_j) = t(t-1)\cdots(t-k)h^{k+1}$$

利用Newton插值(13)得

$$N_n(x_0 + th) = f_0 + t\triangle f_0 + \frac{t(t-1)}{2!}\triangle^2 + \cdots + \frac{t(t-1)\cdots(t-n+1)}{n!}\triangle$$

称为Newton前插公式, 其余项为

$$R_n(x) = \frac{t(t-1)\cdots(t-n)}{(n+1)!}h^{n+1}f^{(n+1)}(\xi), \quad \xi \in (x_0, x_n). \quad (24)$$

当x靠近x_n附近时, 此时将节点重新排列$x_n, x_{n-1}, \cdots, x_1, x_0$, 则有

$$\begin{aligned} N_n(x) &= f(x_n) + f[x_n, x_{n-1}](x - x_n) + f[x_n, x_{n-1}, x_{n-2}](x - x_n)(x - x \\ &+ \cdots + f[x_n, x_{n-1}, \cdots, x_1, x_0](x - x_n)(x - x_{n-1})\cdots(x - x_1). \end{aligned}$$

令$x = x_n + th$, $-1 \le t \le 0$, $\Longrightarrow$

$$N_n(x_n + th) = f_n + t\nabla f_n + \frac{t(t+1)}{2!}\nabla^2$$
$$f_n + \cdots + \frac{t(t+1)\cdots(t+n-1)}{n!}\nabla^n f_n,$$

称为Newton后插公式, 其余项

$$R_n(x) = \frac{t(t+1)\cdots(t+n)}{(n+1)!}h^{n+1}f^{(n+1)}(\xi), \quad \xi \in (x_0, x_n). \quad (25)$$

例4.3

给出$f(x) = \cos x$ 在$x_k = kh, k = 0, 1, \cdots, 6, h = 0.1$处得函数值, 试用4次等距节点插值公式计算$f(0.048)$及$f(0.566)$ 的近似值并估计误差.

4.4 埃尔米特插值(Hermite)

定义4.4

给定$[a,b]$中$n+1$个互异节点x_i $(i=0,1\cdots,n)$上的函数值和直到m_i 阶的导数值$f(x_i), f'(x_i), \cdots, f^{(m_i)}(x_i)$.

令$m=\sum_{i=0}^{n}(m_i+1)-1$, 若存在一个次数不超过$m$的多项式$H_m(x)$, 使得

$$
\begin{array}{ccccccc}
H_m(x_0) & = & f(x_0), H'_m(x_0) & = & f'(x_0), \cdots, H_m^{(m_0)}(x_0) & = & f^{(m_0)}(x_0), \\
H_m(x_1) & = & f(x_1), H'_m(x_1) & = & f'(x_1), \cdots, H_m^{(m_1)}(x_1) & = & f^{(m_1)}(x_1), \\
\vdots & & \vdots & & \vdots & & \\
H_m(x_n) & = & f(x_n), H'_m(x_n) & = & f'(x_n), \cdots, H_m^{(m_n)}(x_n) & = & f^{(m_n)}(x_n),
\end{array}
$$

则称$H_m(x)$为$f(x)$的m次*Hermite*插值多项式.

定理4.4

满足*(26)*的m次多项式$H_m(x)$存在唯一.

证 设$H_m(x)=\sum\limits_{k=0}^{m}c_kx^k$, 代入(26)得

$$
\begin{aligned}
&\sum_{k=0}^{n} c_k x_i^k = f(x_i), \qquad (i=0,1,\cdots,n)\\
&\sum_{k=1}^{n} k c_k x_i^{k-1} = f'(x_i),\\
&\vdots\\
&\sum_{k=m_i}^{n} k(k-1)\cdots(k-m_i+1)c_k x_i^{k-m_i} = f^{(m_i)}(x_i).
\end{aligned}
$$

只要证明上述关于$c_k(k=0,1,\cdots,m)$的线性方程组存在唯一解，或对应的齐次方程组只有零解. 若上述方程右端各项均为零，则x_i为$H_m(x)$ 的m_i+1重根, 因而$H_m(x)$共有$\sum\limits_{i=0}^{n}(m_i+1)=m+1$个零点. 但$H_m(x)$ 是m次多项式，故$H_m(x)$是零多项式，即对应的齐次方程组只有零解.

定理4.5

设$H_m(x)$是满足(26)的m次Hermite插值多项式，$f(x)$在$[a,b]$上具有 m阶连续导数，且在(a,b)内存在$m+1$阶导数. 则对任意$x\in[a,b]$，存在$\xi\in(a,b)$ (ξ依赖与x)使得

$$R_m(x)=f(x)-H_m(x)=\frac{f^{(m+1)}(\xi)}{(m+1)!}\prod_{i=0}^{n}(x-x_i)^{m_i+1}. \qquad (27)$$

Lagrange 型Hermite插值

看一种特殊情况，求一个多项式$H(x)$满足

$$H(x_j) = y_j, \quad H'(x_j) = m_j \quad (j = 0, 1, \cdots, n). \tag{28}$$

插值条件有$2n+2$个，故$H(x)$是$2n+1$次多项式，记为$H_{2n+1}(x)$，按Lagrange插值方法，先求插值基函数$\alpha_j(x)$及$\beta_j(x)$满足

$$\begin{array}{rclrcl} \alpha_j(x_k) & = & \delta_{jk}, & \alpha_j'(x_k) & = & 0; \\ \beta_j(x_k) & = & 0, & \beta_j'(x_k) & = & \delta_{jk}, \end{array} \quad (j, k = 0, 1, \cdots, n). \tag{29}$$

则H_{2n+1}可写成

$$H_{2n+1} = \sum_{j=0}^{m} [y_j \alpha_j(x) + m_j \beta_j(x)]. \tag{30}$$

由条件(29)，显然H_{2n+1}满足(28). 下面求基函数$\alpha_j(x)$和$\beta_j(x)$. 令

$$\alpha_j(x) = (ax+b) l_j^2(x),$$

其中，$l_j(x)$是Lagrange基函数. 由条件(29)得

$$\alpha_j(x_j) = (ax_j + b) l_j^2(x_j) = 1,$$

$$\alpha_j'(x_j) = l_j(x_j)[a l_j(x_j) + 2(ax_j + b) l_j'(x_j)] = 0,$$

整理得

$$a = -2l_j'(x_j), \quad b = 1 + 2x_j l_j'(x_j).$$

而

$$l_j'(x_j) = \sum_{\substack{k=0 \\ k\neq j}}^{n} \frac{1}{x_j - x_k},$$

于是得

$$\alpha_j(x) = \left(1 - 2(x - x_j)\sum_{\substack{k=0 \\ k\neq j}}^{n} \frac{1}{x_j - x_k}\right) l_j^2(x). \tag{31}$$

同理得

$$\beta_j(x) = (x - x_j) l_j^2(x). \tag{32}$$

其误差为

$$R(x) = f(x) - H_{2n+1}(x) = \frac{f^{(2n+2)}(\xi)}{(2n+2)!}\omega_{n+1}^2(x), \tag{33}$$

其中$\xi \in (a, b)$且$\xi \sim x$.

Newton型Hermite插值多项式

考虑下面问题：求线性函数$p(x)$ 满足

$$\begin{cases} p(x_0) = f(x_0), \\ p'(x_0) = f'(x_0). \end{cases} \tag{34}$$

为了解决这个问题，我们先考虑下面的问题：求线性函数$q(x)$满足

$$\begin{cases} q(x_0) = f(x_0), \\ q(x_1) = f(x_1). \end{cases} \tag{35}$$

我们有

$$q(x) = f(x_0) + f[x_0, x_1](x - x_0).$$

令$g(x) = q(x) - f(x)$，则上述条件即为$g(x_0) = 0$，$g(x_1) = 0$，由中值定理知道，存在$\xi \in (x_0, x_1)$使得$g'(\xi) = 0$，即$q'(\xi) = f'(\xi)$ $(\xi \in (x_0, x_1))$. 当$x_1 \to x_0$时，$\xi \to x_0$. 所以在问题(35)中令$x_1 \to x_0$，则该问题就变为问题(34). 从而

$$p(x) = f(x_0) + f[x_0, x_0](x - x_0).$$

从这个例子可以看出，我们可以将插值问题(26)看成是在$m+1$不同节点上的Newton插值，然后取极限就成为$n+1$不同节点上

先推广Newton差商的定义.

定理4.6 (Hermite-Gennochi)

若$f \in C^n[a,b]$, $a \le x_0 < x_1 < \cdots < x_n \le b$, 则有

$$f[x_0, x_1, \cdots, x_n] = \int \underset{\tau_n}{\cdots} \int f^{(n)}(t_0 x_0 + t_1 x_1 + \cdots + t_n x_n) dt_1 \cdots dt_n$$

其中$t_0 = 1 - \sum_{i=1}^{n} t_i$, $\tau_n = \{(t_1, t_2, \cdots, t_n) | t_i \ge 0, \sum_{i=1}^{n} t_i \le 1\}$ 为n维单纯形.

证：用数学归纳法

注意到被积函数是通过一元连续函数$f^{(n)}(x)$与n元线性连续函数$\sum_{i=0}^{n} t_i x_i$ 复合而成，所以$f[x_0, x_1, \cdots, x_n]$是$x_0, x_1, \cdots, x_n$的连续函数．因此

$$f[x_0, x_0] = \lim_{x \to x_0} f[x_0, x] = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0} = f'(x_0),$$

$$\begin{aligned} f[\underbrace{x_0, x_0, \cdots, x_0}_{k+1\text{个}}] &= \lim_{\substack{x_1 \to x_0 \\ \vdots \\ x_k \to x_0}} f[x_0, x_1, \cdots, x_k] \\ &= \lim_{\substack{x_1 \to x_0 \\ \vdots \\ x_k \to x_0}} \frac{f^{(k)}(\eta)}{k!} = \frac{f^{(k)}(x_0)}{k!} \end{aligned}$$

$$f[x_0, x_0, x_1] = \frac{f[x_0, x_1] - f[x_0, x_0]}{x_1 - x_0}.$$

$$
\begin{aligned}
H_m(x) \;=\;& f(x_0) + f[x_0, x_0](x - x_0) + \cdots + f[\underbrace{x_0, \cdots, x_0}_{m_0+1}](x - x_0)^{m_0} \\
& + f[\underbrace{x_0, \cdots, x_0}_{m_0+1}, x_1](x - x_0)^{m_0+1} + \cdots + \\
& f[\underbrace{x_0, \cdots, x_0}_{m_0+1}, \underbrace{x_1, \cdots, x_1}_{m_1+1}](x - x_0)^{m_0+1}(x - x_1)^{m_1} + \cdots + \\
& f[\underbrace{x_0, \cdots, x_0}_{m_0+1}, \cdots, \underbrace{x_{n-1}, \cdots, x_{n-1}}_{m_{n-1}+1}, x_n] \\
& (x - x_0)^{m_0+1} \cdots (x - x_{n-1})^{m_{n-1}+1} \\
& + \cdots + f[\underbrace{x_0, \cdots, x_0}_{m_0+1}, \cdots, \underbrace{x_{n-1}, \cdots, x_{n-1}}_{m_{n-1}+1}, \underbrace{x_n, \cdots, x_n}_{m_n+1}] \\
& (x - x_0)^{m_0+1} \cdots (x - x_{n-1})^{m_{n-1}+1}(x - x_n)^{m_n},
\end{aligned}
$$

插值余项为

$$
\begin{aligned}
f(x) - H_m(x) = \quad & f[\underbrace{x_0, \cdots, x_0}_{m_0+1}, \underbrace{x_1, \cdots, x_1}_{m_1+1}, \cdots, \underbrace{x_n, \cdots, x_n}_{m_n+1}, x] \\
& (x - x_0)^{m_0+1}(x - x_1)^{m_1+1} \cdots (x - x_n)^{m_n+1} \\
= \quad & \frac{f^{(m+1)}(\xi)}{(m+1)!} \prod_{i=0}^{n} (x - x_i)^{m_i+1}
\end{aligned}
$$

其中 $\min(x_0, x_1, \cdots, x_n, x) < \xi < \max(x_0, x_1, \cdots, x_n, x)$.

例4.4

若$n=0, m_0=k$, 即1个$k+1$重节点, 则

$$
\begin{aligned}
H_k(x) &= f(x_0)+f[x_0,x_0](x-x_0)+\cdots+f[\underbrace{x_0,\cdots,x_0}_{k+1}](x-x_0)^k \\
&= f(x_0)+f'(x_0)(x-x_0)+\cdots+\frac{f^{(k)}(x_0)}{k!}(x-x_0)^k.
\end{aligned}
$$

此即为k阶Taylor展开式.

例4.5

求4次Newton型Hermite插值多项式$H(x)$, 使得

$$H(0)=3,\quad H'(0)=4,\quad H(1)=5,\quad H'(1)=6,\quad H''(1)=7.$$

解 可以列表计算各点差商.

k	x_k	$f(x_k)$	1阶差商	2阶差商	3阶差商	4阶差商
0	0	3	4	-2	6	$-\frac{13}{2}$
1	0	3	2	4	$-\frac{1}{2}$	
2	1	5	6	$\frac{7}{2}$		
3	1	5	6			
4	1	5				

所以得

$$H(x)=3+4(x-0)-2(x-0)^2+6(x-0)^2(x-1)-\frac{13}{2}(x-0)^2(x-1)^2.$$

例4.6

设$f(x) \in C^4[a,b]$, 作3次多项式$H_3(x)$, 使得

$$H_3(a) = f(a),\ H_3'(a) = f'(a),\ H_3(b) = f(b),\ H_3'(b) = f'(b)$$

并写出插值余项.

解 由Newton型插值公式得

$$\begin{aligned} H_3(x) &= f(a) + f[a,a](x-a) + f[a,a,b](x-a)^2 \\ &\quad + f[a,a,b,b](x-a)^2(x-b). \end{aligned}$$

求差商.

$$\begin{aligned} f[a,a] &= f'(a), \quad f[b,b] = f'(b), \quad f[a,b] = \frac{f(b)-f(a)}{b-a}, \\ f[a,a,b] &= \frac{f[a,b]-f[a,a]}{b-a} = \frac{f[a,b]-f'(a)}{b-a}, \\ f[a,b,b] &= \frac{f[b,b]-f[a,b]}{b-a} = \frac{f'(b)-f[a,b]}{b-a}, \\ f[a,a,b,b] &= \frac{f[a,b,b]-f[a,a,b]}{b-a} \end{aligned}$$

因而

$$\begin{aligned} H_3(x) &= f(a) + f'(a)(x-a) + \frac{1}{b-a}\{f[a,b] - f'(a)\}(x-a)^2 \\ & \frac{1}{(b-a)^2}\{f'(b) - 2f[a,b] + f'(a)\}(x-a)^2(x-b). \end{aligned}$$

插值余项

$$f(x) - H_3(x) = \frac{f^{(4)}(\xi)}{4!}(x-a)^2(x-b)^2, \quad \xi \in (a,b)$$

4.5 高次插值的缺点及分段低次插值

高次插值的误差分析 n+1个节点，$\max\{|f^{(n)}(x)| \leq M\}$，

$$\max\{|f(x) - L_n(x)|\} \leq \frac{M}{(n+1)!}(b-a)^{n+1}. \tag{36}$$

4.5.1 高次插值的病态性质

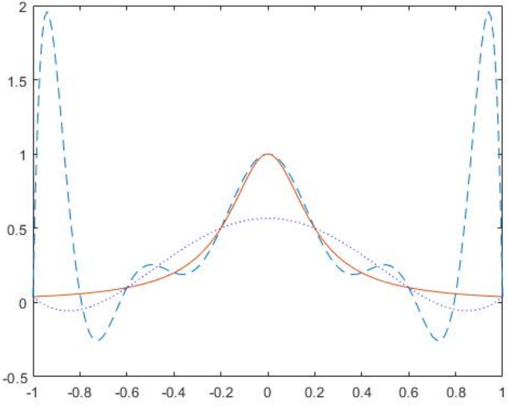
看下面的例子：设$f(x) = 1/(1+25x^2)$，$x \in [-1,1]$，
将$[-1,1]$10等分得节点$x_i = -1 + i/5$ $(i = 0, 1, \cdots, 10)$.
则$f(x)$的10次插值多项式为

$$L_{10}(x) = \sum_{i=0}^{10} f(x_i) l_i(x)$$

其中

$$l_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{10} \frac{x - x_j}{x_i - x_j}.$$

Runger现象



计算结果如下表：

x	$f(x)$	$L_{10}(x)$	x	$f(x)$	$L_{10}(x)$
-1.00	0.03846	0.03848	-0.46	0.15898	0.24145
-0.96	0.04160	1.80438	-0.40	0.20000	0.19999
-0.90	0.04706	1.57872	-0.36	0.23585	0.18878
-0.86	0.05131	0.88808	-0.30	0.30769	0.23535
-0.80	0.05882	0.05882	-0.26	0.37175	0.31650
-0.76	0.06477	-0.20130	-0.20	0.50000	0.50000
-0.70	0.07547	-0.22620	-0.16	0.60976	0.64316
-0.66	0.08410	-0.10832	-0.10	0.80000	0.84340
-0.60	0.10000	0.10000	-0.06	0.91743	0.94090
-0.56	0.11312	0.19873	0.00	1.00000	1.00000
-0.50	0.13793	0.25376			

龙格现象的特征

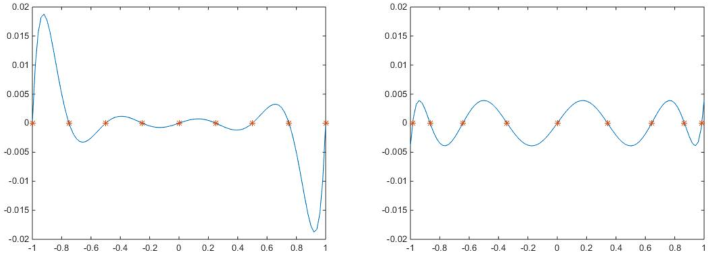
- 多项式$L_{10}(x)$在插值区间的端点附近误差比较大；
- $f(x)$的n次插值多项式$L_n(x)$在$[-1,1]$上不是一致收敛到$f(x)$. $\max|f^{(10)}(x)| \approx 3x10^{13}$.

解决方法：

1. 插值节点往端点处移动；（改变节点的位置以减小$w_{n+1}(x)$的最大值）
2. 尽量不要出现高价导数；

Chebyshev插值

把插值区间固定在$[-1,1]$，多项式插值误差中$W_n(x)=(x-x_1)(x-x_2)\cdots(x-x_n)$是关于$x$的n次多项式，并且在$[-1,1]$上有极值。
目标：在$[-1,1]$上找到特定的节点，使得$W_n(x)$的最大值足够小。



定理4.7

选择实数$-1 \le x_1, \cdots, x_n \le 1$，使得

$$\max_{-1\le x\le 1} |(x-x_1)\cdots(x-x_n)|,$$

尽可能小，则

$$x_i = \cos\frac{(2i-1)\pi}{2n}, i = 1, \cdots, n$$

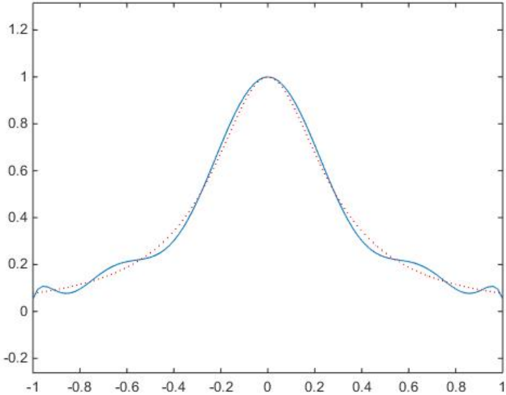
对应的最小值为$1/2^{n-1}$，实际上，通过

$$(x-x_1)\cdots(x-x_n) = \frac{1}{2^{n-1}} T_n(x),$$

可以得到极小值，其中$T_n(x)$表示n阶*Chebyshev*多项式。

选择Chebyshev多项式的零点作为插值节点，在区间$[-1,1]$中请可能均匀地分散了插值误差，这样的插值多项式称为Chebyshew插值多项式。

消除龙格现象



Chebyshev多项式

- $T_n(x) = cos(n \arccos x), (-1 \leq x \leq 1)$,
- 性质：
  1. $T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$, $T_0(x) = 1$, $T_1(x) = x$;
  2. $T_n(x)$是n次多项式；
  3. $T_n(x)$最高处项系数为2^{n-1};
  4. $|T_n(x)| \leq 1$，当$|x| \leq 1$时；
  5. $T_n(x)$在$(-1, 1)$上有n个不同的零点$\cos \dfrac{(2i+1)\pi}{2n}, i = 0, \cdots, n-1$;
  6. $T_n(x) = (-1)^n T_n(-x)$, $T_n(1) = 1$;
  7. $T_n(x)$在-1和1之间一共往返变化$n+1$次；

高阶差分的误差传播

给定函数$f(x)$在一组等距节点上的函数值$f_i = f(x_i) = f(x_0 + ih)$, $i = 0, 1\cdots, n$. 假设在某点x_j处$f(x_j)$有误差ε,即数列$f_0, f_1, \cdots, f_n$变为数列$f_0, f_1, \cdots, f_{j-1}, f_j + \varepsilon, f_{j+1}, \cdots, f_n$,记此数列为$\tilde{f}_0, \tilde{f}_1, \cdots, \tilde{f}_n$, 令$r_i = \tilde{f}_i - f_i$, 则

$$r_i = \begin{cases} \varepsilon, & i = j \\ 0, & i \neq j \end{cases}$$

$$\triangle^k \tilde{f}_i - \triangle^k f_i = \triangle^k r_i.$$

作下面差分表

r_i	$\triangle r_i$	$\triangle^2 r_i$	$\triangle^3 r_i$	$\triangle^4 r_i$	$\triangle^5 r_i$	$\triangle^6 r_i$
0	0	0	ε	-4ε	10ε	-20ε
0	0	ε	-3ε	6ε	-10ε	
0	ε	-2ε	3ε	-4ε		
ε	$-\varepsilon$	ε	$-\varepsilon$			
0	0	0				
0	0					
0						

4.5.2 分段线性插值

给定$f(x)$在$n+1$个节点$a=x_0<x_1<\cdots<x_n=b$上的函数值:

x	x_0	x_1	$\cdots$	x_{n-1}	x_n
$f(x)$	$f(x_0)$	$f(x_1)$	$\cdots$	$f(x_{n-1})$	$f(x_n)$

记$h_i=x_{i+1}-x_i$, $h=\max\limits_{0\le i\le n-1} h_i$. 在每个小区间$[x_i,x_{i+1}]$上作$f(x)$的线性插值

$$L_{1,i}(x)=f(x_i)+f[x_i,x_{i+1}](x-x_i),\quad x\in[x_i,x_{i+1}],$$

其误差为

$$f(x)-L_{1,i}(x)=\frac{1}{2}f''(\xi_i)(x-x_i)(x-x_{i+1}),\quad \xi_i\in(x_i,x_{i+1}),$$

从而有

$$\begin{aligned}\max_{x_i\le x\le x_{i+1}}|f(x)-L_{1,i}(x)| &\le \max_{x_i\le x\le x_{i+1}}\left|\frac{1}{2}f''(\xi_i)(x-x_i)(x-x_{i+1})\right|\\ &\le \frac{1}{8}h_i^2\max_{x_i\le x\le x_{i+1}}|f''(x)|. \qquad (37)\end{aligned}$$

令

$$\tilde{L}_1(x)=\begin{cases} L_{1,0}(x), & x\in[x_0,x_1) \\ L_{1,1}(x), & x\in[x_1,x_2) \\ \vdots & \\ L_{1,n-2}(x), & x\in[x_{n-2},x_{n-1}) \\ L_{1,n-1}(x), & x\in[x_{n-1},x_n], \end{cases}$$

于是有

$$\tilde{L}_1(x_i)=f(x_i)\quad (i=0,1,\cdots,n)$$

即$\tilde{L}_1(x)$是$f(x)$的插值函数, 称为分段线性插值函数,其插值误差为

$$\begin{aligned} \max_{a\le x\le b}|f(x)-\tilde{L}_1(x)| &= \max_{0\le i\le n}\max_{x_i\le x\le x_{i+1}}|f(x)-\tilde{L}_1(x)| \\ &= \max_{0\le i\le n}\max_{x_i\le x\le x_{i+1}}|f(x)-L_{1,i}(x)| \\ &\le \max_{0\le i\le n}\frac{1}{8}h_i^2\max_{x_i\le x\le x_{i+1}}|f''(x)| \\ &\le \frac{1}{8}h^2\max_{a\le x\le b}|f''(x)|. \end{aligned}$$

只要$f(x)$在$[a,b]$上有2阶连续导数, 当$h\to 0$时余项一致趋于零,即分段线性插值函数$\tilde{L}_1(x)$一致收敛于$f(x)$.

4.5.3 分段Hermite插值

给定$f(x)$在$n+1$个节点$a = x_0 < x_1 < \cdots < x_n = b$上的函数表

x	x_0	x_1	$\cdots$	x_{n-1}	x_n
$f(x)$	$f(x_0)$	$f(x_1)$	$\cdots$	$f(x_{n-1})$	$f(x_n)$
$f'(x)$	$f'(x_0)$	$f'(x_1)$	$\cdots$	$f'(x_{n-1})$	$f'(x_n)$

记$h_i = x_{i+1} - x_i$, $h = \max\limits_{0 \le i \le n-1} h_i$. 在每个小区间$[x_i, x_{i+1}]$上利用数据

x	x_i	x_{i+1}
$f(x)$	$f(x_i)$	$f(x_{i+1})$
$f'(x)$	$f'(x_i)$	$f'(x_{i+1})$

作3次Hermite插值

$$
\begin{aligned}
H_{3,i}(x) = \quad & f(x_i) + f'(x_i)(x - x_i) + \frac{f[x_i, x_{i+1}] - f'(x_i)}{h_i}(x - x_i)^2 + \\
& \frac{f'(x_{i+1}) - 2f[x_i, x_{i+1}] + f'(x_i)}{h_i^2}(x - x_i)^2(x - x_{i+1}),
\end{aligned}
$$

其插值余项

$$f(x) - H_{3,i}(x) = \frac{f^{(4)}(\xi)}{4!}(x - x_i)^2(x - x_{i+1})^2, \quad \xi \in (x_i, x_{i+1}).$$

于是

$$\max_{x_i \le x \le x_{i+1}} |f(x) - H_{3,i}(x)| \le \frac{1}{4!}\frac{h_i^4}{16} \max_{x_i \le x \le x_{i+1}} |f^{(4)}(x)|. \tag{38}$$

令

$$\tilde{H}_3(x) = \begin{cases} H_{3,0}(x), & x \in [x_0, x_1) \\ H_{3,1}(x), & x \in [x_1, x_2) \\ \vdots & \\ H_{3,n-2}(x), & x \in [x_{n-2}, x_{n-1}) \\ H_{3,n-1}(x), & x \in [x_{n-1}, x_n]. \end{cases}$$

则

$$\tilde{H}_3(x_i) = f(x_i), \ \tilde{H}_3'(x_i) = f'(x_i) \quad (i = 0, 1, \cdots, n.)$$

即$\tilde{H}_3(x)$满足插值条件.称$\tilde{H}_3(x)$为$f(x)$的分段三次插值函数.

其误差为

$$
\begin{aligned}
\max_{a\le x\le b}|f(x)-\tilde{H}_3(x)| &= \max_{0\le i\le n}\max_{x_i\le x\le x_{i+1}}|f(x)-\tilde{H}_3(x)| \\
&= \max_{0\le i\le n}\max_{x_i\le x\le x_{i+1}}|f(x)-H_{3,i}(x)| \\
&\le \max_{0\le i\le n}\frac{1}{4!}\frac{h_i^4}{16}\max_{x_i\le x\le x_{i+1}}|f^{(4)}(x)| \\
&\le \frac{1}{384}h^4\max_{a\le x\le b}|f^{(4)}(x)|.
\end{aligned}
$$

分段三次Hermite插值的余项和$f(x)$ 的4阶导数有关，当$f(x)$ 在$[a,b]$ 上有4阶连续导数，则有

$$\tilde{H}_3(x)\xrightarrow{\text{一致}}f(x).$$

4.6 三次样条插值

分段插值优点：一致收敛. 缺点：光滑性差.

4.6.1 三次样条插值函数

定义4.5

设在区间$[a,b]$上给定$n+1$个插值节点

$$a = x_0 < x_1 < \cdots < x_n = b$$

及其函数在节点上的值$y_i = f(x_i)$, $i = 0, 1, \cdots, n$. 若存在函数$S(x)$满足：

1. $S(x_j) = y_j,\ j = 0, 1, \cdots, n;$
2. $S(x)$在每个小区间$[x_j, x_{j+1}]$ $j = 0, 1, \cdots, n$上是3次多项式;
3. $S(x) \in C^2[a,b]$.

则称$S(x)$为$f(x)$的3次样条插值函数.

要确定$S(x)$,在每个小区间$[x_j, x_{j+1}]$上要确定4个参数，所以共要确定$4n$个参数. 根据$S(x)$在$[a,b]$上二阶导数连续，在节点x_j, $j=1,2,\cdots,n-1$处满足下面的连续性条件:

$$\begin{aligned} &S(x_j-0)=S(x_j+0), \quad S'(x_j-0)=S'(x_j+0), \\ &S''(x_j-0)=S''(x_j+0). \end{aligned} \tag{39}$$

共有$3n-3$个条件，加上插值条件$n+1$个，共有$4n-2$个条件. 故还要加2个条件. 通常在端点处附加条件(边界条件).常用的边界条件有三种(分别称为第一型，第二型和第三型):

1. 已知两端点的一阶导数，即

$$S'(x_0)=f'(x_0),\ S'(x_n)=f'(x_n). \tag{40}$$

2. 已知两端点的二阶导数，即

$$S''(x_0)=f''(x_0),\ S''(x_n)=f''(x_n). \tag{41}$$

3. 周期边界条件，当$f(x_0)=f(x_n)$时，

$$S'(x_0+0)=S'(x_n-0), \quad S''(x_0+0)=S''(x_n-0). \tag{42}$$

4.6.2 样条插值函数的建立

$S(x)$在$[x_j, x_{j+1}]$上是3次多项式，则$S''(x)$是线性函数，
设$S''(x_j) = M_j$，$S''(x_{j+1}) = M_{j+1}$，则

$$S''(x) = M_j + \frac{1}{h_j}(M_{j+1} - M_j)(x - x_j), \quad x \in [x_j, x_{j+1}] \tag{43}$$

其中$h_j = x_{j+1} - x_j$，$j = 0, 1, \cdots, n-1$. 积分上式得

$$S'(x) = c_j + M_j(x - x_j) + \frac{1}{2h_j}(M_{j+1} - M_j)(x - x_j)^2, \quad x \in [x_j, x_{j+1}]. \tag{44}$$

再积分一次

$$S(x) = y_j + c_j(x - x_j) + \frac{1}{2}M_j(x - x_j)^2 + \frac{1}{6h_j}(M_{j+1} - M_j)(x - x_j)^3, \quad x \in [x_j, x_{j+1}] \tag{45}$$

利用$S(x_{j+1}) = y_{j+1}$，可得

$$c_j = f[x_j, x_{j+1}] - \left(\frac{1}{3}M_j + \frac{1}{6}M_{j+1}\right)h_j, \tag{46}$$

所以

$$\begin{aligned} S(x) = \quad & y_j + \left\{ f[x_j, x_{j+1}] - \left(\frac{1}{3} M_j + \frac{1}{6} M_{j+1} \right) h_j \right\} (x - x_j) \\ & + \frac{1}{2} M_j (x - x_j)^2 + \frac{1}{6h_j} (M_{j+1} - M_j)(x - x_j)^3, \\ & \qquad x \in [x_j, x_{j+1}], \quad j = 0, 1, \cdots, n-1. \end{aligned} \tag{47}$$

由(44)和(46)得

$$\begin{aligned} S'(x_j + 0) = c_j = f[x_j, x_{j+1}] - \left(\frac{1}{3} M_j + \frac{1}{6} M_{j+1} \right) h_j, \\ j = 0, 1, \cdots, n-1, \end{aligned} \tag{48}$$

$$\begin{aligned} S'(x_{j+1} - 0) &= c_j + M_j h_j + \frac{1}{2} (M_{j+1} - M_j) h_j \\ &= f[x_j, x_{j+1}] + \left(\frac{1}{6} M_j + \frac{1}{3} M_{j+1} \right) h_j, \\ & \qquad j = 0, 1, \cdots, n-1. \end{aligned} \tag{49}$$

上式中j换成$j-1$得

$$S'(x_j - 0) = f[x_{j-1}, x_j] + \left(\frac{1}{6}M_{j-1} + \frac{1}{3}M_j\right)h_{j-1},$$
$$j = 1, 2\cdots, n. \tag{50}$$

将(48)和(50)代入连续性方程$S'(x_j - 0) = S'(x_j + 0)$, $j = 1, 2, \cdots, n-1$,

$$\begin{aligned} f[x_{j-1}, x_j] &+ \left(\frac{1}{6}M_{j-1} + \frac{1}{3}M_j\right)h_{j-1} \\ &= f[x_j, x_{j+1}] - \left(\frac{1}{3}M_j + \frac{1}{6}M_{j+1}\right)h_j, \end{aligned}$$

即

$$\mu_j M_{j-1} + 2M_j + \lambda_j M_{j+1} = d_j, \quad j = 1, 2, \cdots, n-1, \tag{51}$$

其中

$$\begin{aligned} \mu_j &= \frac{h_{j-1}}{h_{j-1} + h_j}, \quad \lambda_j = \frac{h_j}{h_{j-1} + h_j} = 1 - \mu_j, \\ d_j &= 6f[x_{j-1}, x_j, x_{j+1}]. \end{aligned} \tag{52}$$

式(51)给出了$n-1$个方程.

第一型 如果边界条件是(40),把$S'(x_0)=f'(x_0)$, $S'(x_n)=f'(x_n)$分别代入(48)和(50)得

$$f[x_0,x_1]-\left(\frac{1}{3}M_0+\frac{1}{6}M_1\right)h_0=f'(x_0),$$
$$f[x_{n-1},x_n]+\left(\frac{1}{6}M_{n-1}+\frac{1}{3}M_n\right)h_{n-1}=f'(x_n),$$

即

$$2M_0+M_1=6f[x_0,x_0,x_1]\equiv d_0, \tag{53}$$
$$M_{n-1}+2M_n=6f[x_{n-1},x_n,x_n]\equiv d_n. \tag{54}$$

联立(51), (53)和(54)得下面的线性方程组

$$\begin{bmatrix} 2 & 1 & & & & \\ \mu_1 & 2 & \lambda_1 & & & \\ & \mu_2 & 2 & \lambda_2 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \mu_{n-1} & 2 & \lambda_{n-1} \\ & & & & 1 & 2 \end{bmatrix} \begin{bmatrix} M_0 \\ M_1 \\ M_2 \\ \vdots \\ M_{n-1} \\ M_n \end{bmatrix} = \begin{bmatrix} d_0 \\ d_1 \\ d_2 \\ \vdots \\ d_{n-1} \\ d_n \end{bmatrix} \tag{55}$$

第二型 如果边界条件是(41), 则得$M_0 = f''(x_0)$, $M_n = f''(x_n)$. 这时(51)的第一个方程和最后一个方程分别为

$$2M_1 + \lambda_1 M_2 = d_1 - \mu_1 f''(x_0), \tag{56}$$

$$\mu_{n-1} M_{n-2} + 2M_{n-1} = d_{n-1} - \lambda_{n-1} f''(x_n). \tag{57}$$

从而得下面线性方程组

$$\begin{bmatrix} 2 & \lambda_1 & & & & \\ \mu_2 & 2 & \lambda_2 & & & \\ & \mu_3 & 2 & \lambda_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \mu_{n-2} & 2 & \lambda_{n-2} \\ & & & & \mu_{n-1} & 2 \end{bmatrix} \begin{bmatrix} M_1 \\ M_2 \\ M_3 \\ \vdots \\ M_{n-2} \\ M_{n-1} \end{bmatrix} = \begin{bmatrix} d_1 - \mu_1 f''(x_0) \\ d_2 \\ d_3 \\ \vdots \\ d_{n-2} \\ d_{n-1} - \lambda_{n-1} f''(x_n) \end{bmatrix}$$

第三型　如果边界条件是(42), 则由$S'(x_0)=S'(x_n)$得

$$\begin{aligned} f[x_0,x_1]-\left(\frac{1}{3}M_0+\frac{1}{6}M_1\right)h_0 &= f[x_{n-1},x_n]+\left(\frac{1}{6}M_{n-1}\right. \\ &\quad \left.+\frac{1}{3}M_n\right)h_{n-1}. \end{aligned} \tag{59}$$

由$S''(x_0)=S''(x_n)$得

$$M_0=M_n$$

代入(59)得

$$\lambda_n M_1+\mu_n M_{n-1}+2M_n=d_n$$

其中

$$\lambda_n=\frac{h_0}{h_0+h_{n-1}},\quad \mu_n=\frac{h_{n-1}}{h_0+h_{n-1}},$$

$$d_n=6\frac{f[x_0,x_1]-f[x_{n-1},x_n]}{h_0+h_{n-1}}.$$

此时(51)的第一个方程为

$$2M_1+\lambda_1 M_2+\mu_1 M_n=d_1,$$

所以得下面的线性方程组

$$\begin{bmatrix} 2 & \lambda_1 & & & & & \mu_1 \\ \mu_2 & 2 & \lambda_2 & & & & \\ & \mu_3 & 2 & \lambda_3 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \mu_{n-2} & 2 & \lambda_{n-2} & \\ & & & & \mu_{n-1} & 2 & \lambda_{n-1} \\ \lambda_n & & & & & \mu_n & 2 \end{bmatrix} \begin{bmatrix} M_1 \\ M_2 \\ M_3 \\ \vdots \\ M_{n-2} \\ M_{n-1} \\ M_n \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \\ d_{n-2} \\ d_{n-1} \\ d_n \end{bmatrix} \quad (60$$

方程(55),(58)和(60)对应的系数矩阵是严格对角占优的, 前2个方程是三对角的, 可以用追赶法求解, 第三个方程也可用类似的方法求解.

求出$M_0, M_1, \ldots, M_n$后, 将他们代入(47)便得三次样条插值函数的分段表达式.

例4.7

给定数据：

x	1	2	4	5
$f(x)$	1	3	4	2

求$f(x)$的自然(边界条件)3次样条插值函数，并求$f(3)$和$f(4.5)$的近似值.

解 记$x_0=1\ x_1=2,\ x_2=4,\ x_3=5$，则

$$f(x_0)=1,\ f(x_1)=3,\ f(x_2)=4,\ f(x_3)=2$$
$$h_0=x_1-x_0=1,\ h_1=x_2-x_1=2,\ h_3=x_3-x_2=1$$
$$\mu_1=\frac{h_0}{h_0+h_1}=\frac{1}{3},\ \mu_2=\frac{h_1}{h_1+h_2}=\frac{2}{3}$$
$$f[x_0,x_1,x_2]=-\frac{1}{2},\ f[x_1,x_2,x_3]=-\frac{5}{6}.$$

由自然边界条件知$M_0 = M_3 = 0$, 故得线性方程组

$$\begin{bmatrix} 2 & \frac{2}{3} \\ \frac{2}{3} & 2 \end{bmatrix} \begin{bmatrix} M_1 \\ M_2 \end{bmatrix} = 6 \begin{bmatrix} -\frac{1}{2} \\ -\frac{5}{6} \end{bmatrix}$$

解得$M_1 = -\dfrac{3}{4},\ M_2 = -\dfrac{9}{4}$.代入(47)得3次样条函数

$$S(x) = \begin{cases} 1 + \frac{17}{8}(x-1) - \frac{1}{8}(x-1)^3, & 1 \le x < 2, \\ 3 + \frac{7}{4}(x-2) - \frac{3}{8}(x-2)^2 - \frac{1}{8}(x-2)^3, & 2 \le x < 4, \\ 4 - \frac{5}{4}(x-4) - \frac{9}{8}(x-4)^2 + \frac{3}{8}(x-4)^3, & 4 \le x \le 5. \end{cases}$$

计算$f(3) \approx S(3) = \dfrac{17}{4},\ f(4.5) \approx S(4.5) = \dfrac{201}{64}$.

4.6.3　3次样条函数的误差界

设$g(x) \in C[a,b]$，记

$$\|g\|_\infty = \max_{a \le x \le b} |g(x)|.$$

定理4.8

设$f(x) \in C^4[a,b]$,$S(x)$为满足第一边界条件(40)或第二边界条件(41) 的3次样条函数，$h = \max\limits_{0 \le i \le n-1} h_i$，$h_i = x_{i+1} - x_i$ $(i = 0, 1, \cdots, n-1)$，则有估计

$$\|f^{(k)} - S^{(k)}\|_\infty \le c_k \|f^{(4)}\|_\infty h^{4-k}, k = 0, 1, 2, \tag{61}$$

其中$c_0 = \dfrac{1}{16}$，$c_1 = c_2 = \dfrac{1}{2}$.

4.7 最佳一致逼近

4.7.1　线性赋范空间

定义4.6 (线性空间)

设X是一个集合. 如果对$\forall x, y \in X, \lambda \in R$, 有$\lambda x \in X, x + y \in X$, 则称$X$是线性空间.

定义4.7

设X是一个线性空间. 若对$\forall x \in X$, 对应于实数, 记为$\|x\|$, 且满足下面关系:

1. $\forall x \in X$, 有$\|x\| \geq 0$, 且$\|x\| = 0 \Longleftrightarrow x = 0$.
2. $\forall \lambda \in R, x \in X$, 有$\|\lambda x\| = |\lambda| \|x\|$.
3. $\forall x, y \in X$, 有$\|x + y\| \leq \|x\| + \|y\|$.

则称$\|\cdot\|$为X上的一个范数, 对应的空间称线性赋范空间.

定义4.8

设X是线性赋范空间, $x, y \in X$, 称$\|x - y\|$为x和y之间的距离.

例　当$X = R^n$时, 即为向量范数, 有$1, 2, \infty$范数.

例　$X = C[a, b] = \{f | f(x)在[a, b]上连续\}$. 在$C[a, b]$上定义通常的加法和数乘运算后$C[a, b]$是一个线性空间.

设$f \in C[a,b]$, 记

$$\|f\|_1 = \int_a^b |f(x)|\,dx, \quad \|f\|_\infty = \max_{a\le x\le b} |f(x)|,$$
$$\|f\|_2 = \sqrt{\int_a^b [f(x)]^2\,dx}.$$

则$\|\cdot\|_1, \|\cdot\|_\infty, \|\cdot\|_2$是$C[a,b]$上的范数.
设$f, g \in C[a,b]$, f和g在$[a,b]$上的最大误差表示为:

$$\|f-g\|_\infty = \max_{a\le x\le b} |f(x)-g(x)|.$$

定义4.9
设X是线性赋范空间, $M \subseteq X$是X的子空间, $f \in X$.
若$\exists \varphi \in M$使$\forall \psi \in M$有

$$\|f-\varphi\| \le \|f-\psi\|,$$

则称φ是f在M中的最佳逼近元.

4.7.2 最佳一致逼近多项式

记$M_n = \{p_n | p_n$为次数不超过n的多项式$\}$, 则$M_n \subset C[a, b]$.

定义4.10

设$f \in C[a, b]$. 若$\exists p_n \in M_n$, 使得对$\forall q_n \in M_n$, 有

$$\|f - p_n\|_\infty \le \|f - q_n\|_\infty.$$

则称$p_n(x)$是$f(x)$的n次最佳一致逼近多项式.

注 由定义知

$$\|f - p_n\|_\infty = \min_{q_n \in M_n} \|f - q_n\|_\infty.$$

或

$$\max_{a \le x \le b} |f(x) - p_n(x)| = \min_{q_n \in M_n} \max_{a \le x \le b} |f(x) - q_n(x)|.$$

最佳一致逼近多项式是否存在、唯一性以及如何构造？

定理4.9 (存在性)

设$f \in C[a,b]$, 则f在M_n中存在n次最佳一致逼近多项式$p_n(x)$.

Proof.

定义多元函数

$$\varphi(a_0, a_1, \cdots, a_n) = \max_{a \le x \le b} |f(x) - \sum_{k=0}^{n} a_k x^k| \tag{62}$$

以下证明两件事情：

1. $\varphi(x)$在R^{n+1}上连续；
2. 构造一个有界闭区域D,使得

$$\min_{x \in D} \varphi(x) = \min_{x \in R^{n+1}} \varphi(x).$$

$\square$

最佳一致逼近多项式的特征

定义4.11

设$g \in C[a,b]$. 如果$\exists x_0 \in [a,b]$使得$|g(x_0)| = \|g\|_\infty = \max_{a\le x\le b}|g(x)|$, 则称$x_0$为$g(x)$在$[a,b]$上的偏差点.

当$g(x_0) = \|g\|_\infty$, x_0称$g(x)$的正偏差点.

当$g(x_0) = -\|g\|_\infty$, x_0称$g(x)$的负偏差点.

引理4.1

设$f \in C[a,b]$, $p_n(x)$是$f(x)$的n次最佳一致逼近多项式,
则$f - p_n$必存在正负偏差点.

近似最佳一致逼近多项式

$f(x)$定义在[-1,1]上的函数，并设$f(x)$具有$n+1$阶连续导数$f^{(n+1)}(x)$.作n次插值多项式

$$L_n(x) = \sum_{i=0}^{n} f(x_i)\Pi_{j=0,j\neq i}^{n} \frac{x-x_j}{x_i-x_j},$$

则插值余项为

$$f(x) - L_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} W_{n+1}(x).$$

其中$W_{n+1}(x) = \Pi_{i=0}^{n}(x-x_i)$
因为$W_{n+1}(x)$是n+1次首1多项式，为了使其在$[-1,1]$上的无穷范数$\|W_{n+1}(x)\|_\infty$最小，插值点应取n+1次Chebyshev多项式$T_{n+1}(x)$的零点$x_i = \cos\frac{(2i+1)\pi}{2n+2}, (i = 0, 1, \cdots, n)$,

$$\max_{-1\leq x\leq 1} |f(x) - L_n(x)| \leq \frac{\max_{-1\leq x\leq 1} |f^{(n+1)}(x)|}{(n+1)!} \max_{-1\leq x\leq 1} |W_{n+1}(x)| \quad (63)$$

例4.8

设$f(x)=xe^x, x\in[0,1.5]$,求$f(x)$的3次近似最佳一致逼近多项式。

解: 作变换$x=0.75+0.75t$, 由4次Chebyshev多项式$T_4(t)$的4个零点$\cos\left(i+\frac{1}{2}\right)\frac{\pi}{4}(i=0,1,2,3)$得到4个插值节点为

$$
\begin{aligned}
x_0 &= 0.75+0.75\cos\frac{\pi}{8}=1.44291,\\
x_1 &= 0.75+0.75\cos\frac{3\pi}{8}=1.03701,\\
x_2 &= 0.75+0.75\cos\frac{5\pi}{8}=0.46299,\\
x_3 &= 0.75+0.75\cos\frac{7\pi}{8}=0.05709,
\end{aligned}
$$

x_k	$f(x_k)$	$f[x_k, x_{k+1}]$	$f[x_k, x_{k+1}, x_{k+2}]$	$f[x_k, x_{k+1}, x_{k+2}, x_{k+3}]$
1.44291	6.10783	7.84100	4.10908	1.38110
1.03701	2.92517	3.81443	2.19512	
0.46299	0.73561	1.66339		
0.05709	0.06044			

3次近似最佳一致逼近多项式为

$$\begin{aligned} N_3(x) &= 6.10783 + 7.84100(x - 1.44291) \\ &\quad +4.10908(x - 1.44291)(x - 1.03701) \\ &\quad +1.38110(x - 1.44291)(x - 1.03701)(x - 0.46299) \end{aligned}$$

插值余项估计

$$|f(x) - N_3(x)| \leq \left(\frac{1.5 - 0}{2}\right)^4 \frac{2^{-3}}{4!} \max_{0 \leq x \leq 1.5} |f^{(4)}(x)| = 0.040621 \tag{64}$$

4.8 最佳平方逼近

4.8.1 内积空间

定义5.1

设X是一个线性空间，若对$\forall x, y \in X$有实数与之对应，记该实数为(x, y)，且满足:

1. $\forall x, y \in X$，有$(x, y) = (y, x)$;
2. $\forall x, y \in X, \lambda \in \mathbf{R}$，有$(\lambda x, y) = \lambda(x, y)$;
3. $\forall x, y, z \in X$，有$(x + y, z) = (x, z) + (y, z)$;
4. $\forall x \in X$，有$(x, x) \geq 0$，且$(x, x) = 0 \Longleftrightarrow x = 0$.

则X称为内积空间，二元运算$(\cdot, \cdot)$称为内积.

定义5.2

设X是内积空间，$x, y \in X$，如果$(x, y) = 0$，则称x和y正交.

例 $X=\mathbf{R}^n$, $x=(x_1,x_2,\cdots,x_n)^T$, $y=(y_1,y_2,\cdots,y_n)^T$, 记

$$(x,y)=\sum_{i=1}^{n}x_iy_i,$$

则(x,y)是$\mathbf{R}^n$上的一个内积.

例 考虑线性空间$C[a,b]$. 对$f,g\in C[a,b]$, 记

$$(f,g)=\int_a^b f(x)g(x)dx,$$

则(f,g)为$C[a,b]$中的一个内积.

引理5.1 (Cauchy-Schwartz 不等式)

设X是一个内积空间, 则对 $\forall x,y\in X$ 有

$$(x,y)^2\leq(x,x)(y,y).$$

设X是一个内积空间, $x\in X$, 定义

$$\|x\|=\sqrt{(x,x)},$$

则可以验证$\|x\|$是X上的一个范数, 称为2范数.

4.8.2 最佳平方逼近

设X是内积空间，$(\cdot,\cdot)$是内积，M是X的有限维子空间，φ_0，φ_1，$\cdots$，φ_m 是M的一组基，$f\in X$，求$\varphi\in M$使得

$$\|f-\varphi\|\leq\|f-\psi\|,\quad\forall\psi\in M,\tag{65}$$

或者

$$\|f-\varphi\|=\min_{\psi\in M}\|f-\psi\|.$$

记$\varphi=\sum_{i=0}^{m}c_i\varphi_i$，$\psi=\sum_{i=0}^{m}a_i\varphi_i$，则问题(65)即求$c_0,c_1,\cdots,c_m$使得

$$(f-\sum_{i=0}^{m}c_i\varphi_i,f-\sum_{j=0}^{m}c_j\varphi_j)=\min_{\psi\in M}(f-\sum_{i=0}^{m}a_i\varphi_i,f-\sum_{j=0}^{m}a_j\varphi_j).$$

记

$$\Phi(a_0,a_1,\cdots,a_m)=(f-\sum_{i=0}^{m}a_i\varphi_i,f-\sum_{j=0}^{m}a_j\varphi_j),$$

则即求$c_0,c_1,\cdots,c_m$使得

$$\Phi(c_0,c_1\cdots,c_m)=\min_{a_0,a_1,\cdots,a_m\in\mathbf{R}}\Phi(a_0,a_1,\cdots,a_m).$$

令

$$\frac{\partial \Phi}{\partial a_k} = -2(f, \varphi_k) + 2\sum_{i=0}^{m} a_i(\varphi_i, \varphi_k) = 0, \quad k = 0, 1, \cdots, m.$$

即

$$\sum_{i=0}^{m} (\varphi_k, \varphi_i) a_i = (f, \varphi_k), \quad k = 0, 1, \cdots, m. \tag{66}$$

所以$c_0, c_1, \cdots, c_m$是方程(66)的解. 易证方程(66)的系数矩阵是对称正定矩阵, 故有唯一解.

4.8.3 离散数据的最佳平方逼近

定义5.3

给定数据

x	x_1	x_2	x_3	$\cdots$	x_n
y	y_1	y_2	y_3	$\cdots$	y_n

设$\varphi_0(x), \varphi_1(x), \cdots, \varphi_m(x)$线性无关. 令

$$p(x) = \sum_{i=0}^{m} c_i \varphi_i(x), \quad q(x) = \sum_{i=0}^{m} a_i \varphi_i(x),$$

$$\Phi(a_0, a_1, \cdots, a_m) = \sum_{k=1}^{n} (q(x_k) - y_k)^2,$$

求$c_0, c_1, \cdots, c_m$, 使得

$$\Phi(c_0, c_1, \cdots, c_m) = \min_{a_0, a_1, \cdots, a_m \in \mathbf{R}} \Phi(a_0, a_1, \cdots, a_m). \tag{67}$$

称$p(x)$为数据的拟合函数.

如果$\varphi_k(x) = x^k$, 则称$p(x)$为m次最小二乘多项式. 记

$$\varphi_k = \begin{bmatrix} \varphi_k(x_1) \\ \varphi_k(x_2) \\ \vdots \\ \varphi_k(x_n) \end{bmatrix}, \quad k = 0, 1, \cdots, m, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

则$c_0, c_1, \cdots, c_m$是下面的线性方程组的解.

$$\begin{bmatrix} (\varphi_0, \varphi_0) & (\varphi_0, \varphi_1) & \cdots & (\varphi_0, \varphi_m) \\ (\varphi_1, \varphi_0) & (\varphi_1, \varphi_1) & \cdots & (\varphi_1, \varphi_m) \\ \vdots & \vdots & \vdots & \vdots \\ (\varphi_m, \varphi_0) & (\varphi_m, \varphi_1) & \cdots & (\varphi_m, \varphi_m) \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_m \end{bmatrix} = \begin{bmatrix} (\mathbf{y}, \varphi_0) \\ (\mathbf{y}, \varphi_1) \\ \vdots \\ (\mathbf{y}, \varphi_m) \end{bmatrix}$$

例5.1

观察物体的直线运动，得到如下数据：

t	0	0.9	1.9	3.0	3.9	5.0
s	0	10	30	51	80	111

试用最小二乘法求2次多项式$f(t) = c_0 + c_1 t + c_2 t^2$拟合上述数据.

解 $\varphi_0(t) = 1, \varphi_1(t) = t, \varphi_2(t) = t^2.$

$$\varphi_0 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \varphi_1 = \begin{bmatrix} 0 \\ 0.9 \\ 1.9 \\ 3.0 \\ 3.9 \\ 5.0 \end{bmatrix}, \quad \varphi_2 = \begin{bmatrix} 0 \\ 0.81 \\ 3.61 \\ 9 \\ 15.21 \\ 25 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 0 \\ 10 \\ 30 \\ 51 \\ 80 \\ 111 \end{bmatrix},$$

代入方程(68)得

$$\begin{bmatrix} 6 & 14.7 & 53.63 \\ 14.7 & 53.63 & 218.907 \\ 53.63 & 218.907 & 951.0323 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 282 \\ 1086 \\ 4567.2 \end{bmatrix}$$

解得$c_0 = -0.6170, c_1 = 11.1586, c_2 = 2.2687.$

4.8.4 超定线性方程组的最小二乘解

给定方程组

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix} \tag{68}$$

其中$m > n$, 系数矩阵$\mathbf{A}$的列向量线性无关. 方程(68)称为超定方程组. 该方程组一般没有精确解. 记

$$\mathbf{A}_j = \begin{bmatrix} a_{1j} \\ a_{2j} \\ \vdots \\ a_{mj} \end{bmatrix}, \quad j = 1, 2 \cdots, n, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix},$$

则

$$\mathbf{A} = (\mathbf{A}_1, \mathbf{A}_2, \cdots, \mathbf{A}_n).$$

方程组(68)可写为

$$x_1\mathbf{A}_1 + x_2\mathbf{A}_2 + \cdots + x_n\mathbf{A}_n = \mathbf{b}.$$

记$\mathbf{M} = \mathrm{span}\{\mathbf{A}_1, \mathbf{A}_2, \cdots, \mathbf{A}_n\}$, 则$\mathbf{M}$是$\mathbf{R}^m$的一个有限维子空间.
记

$$\Phi(x_1, x_2, \cdots, x_n) = \|\mathbf{b} - \sum_{i=1}^{n} x_i \mathbf{A}_i\|^2,$$

求$x_1^*, x_2^*, \cdots, x_n^*$, 使得

$$\Phi(x_1^*, x_2^*, \cdots, x_n^*) = \min_{x_1, x_2, \cdots, x_n \in \mathbf{R}} \Phi(x_1, x_2, \cdots, x_n).$$

由2节理论知, $x_1^*, x_2^*, \cdots, x_n^*$是下面方程组的解:

$$\begin{bmatrix} (\mathbf{A}_1, \mathbf{A}_1) & (\mathbf{A}_1, \mathbf{A}_2) & \cdots & (\mathbf{A}_1, \mathbf{A}_n) \\ (\mathbf{A}_2, \mathbf{A}_1) & (\mathbf{A}_2, \mathbf{A}_2) & \cdots & (\mathbf{A}_2, \mathbf{A}_n) \\ \vdots & \vdots & \vdots & \vdots \\ (\mathbf{A}_n, \mathbf{A}_1) & (\mathbf{A}_n, \mathbf{A}_2) & \cdots & (\mathbf{A}_n, \mathbf{A}_n) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} (\mathbf{b}, \mathbf{A}_1) \\ (\mathbf{b}, \mathbf{A}_2) \\ \vdots \\ (\mathbf{b}, \mathbf{A}_n) \end{bmatrix},$$

即

$$\mathbf{A}^T \mathbf{A} \mathbf{x} = \mathbf{A}^T \mathbf{b}$$

例5.2

求下列超定方程组的最小二乘解:

$$\begin{cases} 3x+4y &= 5 \\ -4x+8y &= 1 \\ 6x+3y &= 3 \end{cases}$$

解 系数矩阵和右端向量为

$$\mathbf{A}=\begin{bmatrix} 3 & 4 \\ -4 & 8 \\ 6 & 3 \end{bmatrix},\quad \mathbf{b}=\begin{bmatrix} 5 \\ 1 \\ 3 \end{bmatrix},$$

$$\mathbf{A}^T\mathbf{A}=\begin{bmatrix} 61 & -2 \\ -2 & 89 \end{bmatrix},\quad \mathbf{A}^T\mathbf{b}=\begin{bmatrix} 29 \\ 37 \end{bmatrix},$$

得方程组

$$\begin{bmatrix} 61 & -2 \\ -2 & 89 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix}=\begin{bmatrix} 29 \\ 37 \end{bmatrix},$$

解得$x=0.4894, y=0.4267.$

4.8.5 连续函数的最佳平方逼近

设$f(x)\in C[a,b]$，$M=\mathrm{span}\{\varphi_0(x),\varphi_1(x),\cdots,\varphi_m(x)\}$是$C[a,b]$的一个$m+1$维子空间. $q(x),p(x)\in M$可表示为

$$q(x)=\sum_{i=0}^{m}a_i\varphi_i(x),\quad p(x)=\sum_{i=0}^{m}c_i\varphi_i(x).$$

记

$$\Phi(a_0,a_1,\cdots,a_m)=\|f-q\|^2=\int_a^b[f(x)-\sum_{i=0}^{m}a_i\varphi_i(x)]^2dx.$$

求$c_0,c_1,\cdots,c_m$使得

$$\|f-p\|_2\le\|f-q\|_2,\quad\forall q\in M.$$

即

$$\Phi(c_0,c_1,\cdots,c_m)=\min_{a_0,a_1,\cdots,a_m\in\mathbf{R}}\Phi(a_0,a_1,\cdots,a_m).$$

由2节最佳平方逼近理论, $c_0, c_1, \cdots, c_m$是下面的(正规)方程组的解:

$$\begin{bmatrix} (\varphi_0,\varphi_0) & (\varphi_0,\varphi_1) & \cdots & (\varphi_0,\varphi_m) \\ (\varphi_1,\varphi_0) & (\varphi_1,\varphi_1) & \cdots & (\varphi_1,\varphi_m) \\ \vdots & \vdots & \vdots & \vdots \\ (\varphi_m,\varphi_0) & (\varphi_m,\varphi_1) & \cdots & (\varphi_m,\varphi_m) \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_m \end{bmatrix} = \begin{bmatrix} (f,\varphi_0) \\ (f,\varphi_1) \\ \vdots \\ (f,\varphi_m) \end{bmatrix}, (69)$$

其中

$$(\varphi_i,\varphi_j) = \int_a^b \varphi_i(x)\varphi_j(x)dx,\ (f,\varphi_i) = \int_a^b f(x)\varphi_i(x)dx.$$

如果$\varphi_i(x) = x^i (i = 0, 1\cdots, m)$, 则$p(x)$称为$f(x)$在$[a, b]$上的$m$次最佳平方逼近多项式.

例5.3

设$f(x)=e^x, x\in[0,1]$. 求$f(x)$的2次最佳平方逼近多项式$p_2(x)=c_0+c_1x+c_2x^2$.

解 $\varphi_0(x)=1, \varphi_1(x)=x, \varphi_2(x)=x^2$,

$$(\varphi_0,\varphi_0)=\int_0^1 1dx, \quad (\varphi_0,\varphi_1)=\int_0^1 xdx=\frac{1}{2},$$

$$(\varphi_0,\varphi_2)=\int_0^1 x^2dx=\frac{1}{3}, \quad (\varphi_1,\varphi_1)=\int_0^1 x^2=\frac{1}{3},$$

$$(\varphi_1,\varphi_2)=\int_0^1 x^3dx=\frac{1}{4}, \quad (\varphi_2,\varphi_2)=\int_0^1 x^4dx=\frac{1}{5},$$

$$(f,\varphi_0)=\int_0^1 e^xdx=e-1, \quad (f,\varphi_1)=\int_0^1 xe^xdx=1,$$

$$(f,\varphi_2)=\int_0^1 x^2e^xdx=e-2.$$

正规方程组为:

$$\begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} e-1 \\ 1 \\ e-2 \end{bmatrix}.$$

解得$c_0 = 39e - 105, c_1 = 588 - 216e, c_2 = 210e - 570.$
$f(x)$的2次最佳平方逼近多项式为

$$\begin{aligned} p_2(x) &= 39e - 105 + (588 - 216e)x + (210e - 570)x^2 \\ &\approx 1.0130 + 0.8515x + 0.8392x^2. \end{aligned}$$

例5.4

求c, d, 使得

$$\int_0^1 \left[x^3 - c - dx^2\right]^2 dx$$

取最小值.

解 该问题即求$f(x) = x^3$在$[0,1]$上的最佳平方逼近多项式$p(x) = c + dx^2$. $\varphi_0(x) = 1, \varphi_1(x) = x^2$.

$$(\varphi_0, \varphi_0) = \int_0^1 1dx = 1, \quad (\varphi_0, \varphi_1) = \int_0^1 x^2 = \frac{1}{3},$$

$$(\varphi_1, \varphi_1) = \int_0^1 x^4 dx = \frac{1}{5}, \quad (f, \varphi_0) = \int_0^1 x^3 dx = \frac{1}{4},$$

$$(f, \varphi_2) = \int_0^1 x^5 dx = \frac{1}{6}.$$

正规方程为:

$$\begin{bmatrix} 1 & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{5} \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix} = \begin{bmatrix} \frac{1}{4} \\ \frac{1}{6} \end{bmatrix}. \Rightarrow c = -\frac{1}{16}, d = \frac{15}{16}$$

解得$c = -\frac{1}{\ }, d = \frac{15}{\ }$