函数的近似方法
—常用的插值法与基于最小二乘法的拟合法

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Outline

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公邮or 微信

课件及讨论通过 “新 计算物理”联系方式来进行交流.

作业也可发到

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上节课的回顾

- Matlab基本特点及简单应用
  基于矩阵
  help name
- 程序设计的基本特点
  程序设计的基本结构：顺序、循环、分支等;
- 如何体现物理特点
  如何控制程序，写程序一定要理解公式的物理含义。

定义

假设一组观测点和对就的测量值之间的列表如下，

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

假定满足的函数关系为

$$y_i(x) = y(x_i), i = 1, 2, \cdots, n$$

根据这个对应关系寻求$y(x_i)$的一个近似函数关系$f(x_i)$，得到的$f(x)$称为插值函数，x_i称为插值点(或节点)。插值函数在插值点要满足的最基本条件是：

1. 在插值点x_i $(i = 1, 2, \cdots, n)$上，要求插值函数$f(x_i)$的值与插值y_i相等；
2. 在插值点一阶导数连续，甚至二阶导连续；
3. 对于m次插值多项式，要求有$m+1$个插值条件，以唯一确定$m+1$个系数。

两点一次插值

在两插值点$[x_i,y_i]$和 $[x_{i+1}, y_{i+1}]$用直线连接，在区间$[x_i, x_{i+1}]$内构造的线性插值函数为

$$y = f(x) = ax + b$$

系数可由两个插值点确定

$$f(x_i) = ax_i + b = y_i, \quad f(x_{i+1}) = ax_{i+1} + b = y_{i+1}$$

得插值函数

$$y(x) = \frac{x - x_{i+1}}{x_i - x_{i+1}} y(x_i) + \frac{x - x_i}{x_{i+1} - x_i} y(x_{i+1}), x_i \le x \le x_{i+1}$$

$$f(x) = l_i(x) f(x_i) + l_{i+1}(x) f(x_{i+1})$$

上式被称为拉格朗日一次插值多项式。

两点二次插值

对于两个插值点$[x_i,y_i]$和$[x_{i+1},y_{i+1}]$,在此区间内构造二次函数$y=f(x)=ax^2+bx+c$,系数a,b,c的确定方法二个插值点及其左端一阶导数连续为条件，$i.e.$

$$
\begin{aligned}
f(x_i) &= ax_i^2+bx_i+c=y_i\\
f(x_{i+1}) &= ax_{i+1}^2+bx_{i+1}+c=y_{i+1}\\
f'(x_i) &= y_i'; 2ax_i+b=y'
\end{aligned}
$$

容易得到

$$f(x)=a(x-x_i)^2+y_i'(x-x_i)+y_i, a=\frac{\Delta y_i-y_i'\Delta x_i}{(\Delta x_i)^2}$$

其中，$\Delta y_i=y_{i+1}-y_i, \Delta x_i=x_{i+1}-x_i$.

三点抛物线插值

给定三个插值点$(x_{i-1},y(x_{i-1}))$, $(x_i,y(x_i))$, and $(x_{i+1},y(x_{i+1}))$, 假定过三个节点的三次插值函数为,

$$y(x) = a + bx + cx^2$$

由三个节点可求得 a, b and c, 得三点插值函数

$$y(x) = l_{i-1}(x)y(x_{i-1}) + l_i(x)y(x_i) + l_{i+1}(x)y(x_{i+1})$$

$$x_{i-1} \leq x \leq x_{i+1}$$

$$\begin{aligned}
l_{i-1}(x) &= \frac{(x-x_i)(x-x_{i+1})}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})} \\
l_i(x) &= \frac{(x-x_{i-1})(x-x_{i+1})}{(x_i-x_{i-1})(x_i-x_{i+1})} \\
l_{i+1} &= \frac{(x-x_{i-1})(x_-x_i)}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)}
\end{aligned}$$

上式被称为拉格朗日二次插值多项式，也称为抛物线插值.

$n+1$点n次插值

采用逐次线性插值方法可以构造出高次的插值多项式。定义$y_{i,i+1,\cdots,i+m}$为通过$m+1$个节点(x_i, y_i), (x_{i+1}, y_{i+1})的m次插值多项式，有关系

$$y_{i,i+1,\cdots,i+m}(x) = \frac{x - x_{i+m}}{x_i - x_{i+m}} y_{i,i+1,\cdots,i+m-1}(x) + \frac{x - x_i}{x_{i+m} - x_i} y_{i+1,i+2,\cdots,i+m}(x)$$

或记为

$$y_{i\cdots j} = \frac{x - x_j}{x_i - x_j} y_{i\cdots j-1} + \frac{x - x_i}{x_j - x_i} y_{i+1\cdots j}$$

例如：

$$\begin{aligned} y_{123} &= \frac{x - x_3}{x_1 - x_3} y_{12} + \frac{x - x_1}{x_3 - x_1} y_{23} = \frac{x - x_3}{x_1 - x_3} \left(\frac{x - x_2}{x_1 - x_2} y_1 + \frac{x - x_1}{x_2 - x_1} y_2\right) \\ &\quad \frac{x - x_1}{x_3 - x_1} \left(\frac{x - x_3}{x_2 - x_3} y_2 + \frac{x - x_2}{x_3 - x_2} y_3\right) \\ &= \left(\frac{x - x_3}{x_1 - x_3} \frac{x - x_2}{x_1 - x_2}\right) y_1 + \left(\frac{x - x_3}{x_2 - x_3} \frac{x - x_1}{x_2 - x_1}\right) y_2 + \left(\frac{x - x_1}{x_3 - x_1} \frac{x - x_2}{x_3 - x_2}\right) y_3 \end{aligned}$$

为三点插值公式.

5个插值点的逐次线性插值

$$y_{12345} = \frac{x - x_5}{x_1 - x_5} y_{1234} + \frac{x - x_1}{x_5 - x_1} y_{2345}$$

$$\begin{array}{cccccc}
x_1 & y_1 & & & & \\
 & & y_{12} & & & \\
x_2 & y_2 & & y_{123} & & \\
 & & y_{23} & & y_{1234} & \\
x_3 & y_3 & & y_{234} & & y_{12345} \\
 & & y_{34} & & y_{2345} & \\
x_4 & y_4 & & y_{345} & & \\
 & & y_{45} & & & \\
x_5 & y_5 & & & &
\end{array}$$

多项式插值：
设已知函数$f(x)$在区间[a,b]的$n+1$个点

$$a = x_0 < x_1 < x_2 < \cdots < x_i < \cdots < x_n = b$$

的函数值为

$$y_k = f(x_k), k = 0, 1, 2, \cdots, n$$

采用多项式

$$P(x) = a_0 x^n + a_1 x^{n-1} + \cdots + a_{n-1} x + a_n$$

$a_0, a_1, \cdots, a_n$为待定系数，$p(x)$满足条件

$$p(x) = y_0 l_0(x) + y_1 l_1(x) + \cdots + y_n l_n(x)$$

$l_0(x), l_1(x), \cdots, l_n(x)$满足下列条件

$$l_i(x) = \begin{cases} 1 & x = x_j \quad i = j \\ 0 & x = x_j \quad i \neq j \end{cases}$$

因此,

$$p(x_i) = y_i, i = 0, 1, \cdots, n.$$

$$\frac{w(x_0, x_1, \cdots, x_{i-1}, x, x_{i+1}, \cdots, x_n)}{w(x_0, x_1, \cdots, x_{i-1}, x_i, x_{i+1}, \cdots, x_n)} = \begin{cases} 1 & x = x_j \quad i = j \\ 0 & x = x_j \quad i \neq j \end{cases}$$

Lagrange polynomials are defined as

$$L_i(x) = \frac{(x - x_0)\cdots(x - x_{i-1})(x - x_{i+1})\cdots(x - x_n)}{(x_i - x_0)\cdots(x_i - x_{i-1})(x_i - x_{i+1})\cdots(x_i - x_n)}$$

$$p(x) = \sum_{i=0}^{n} f_i L_i(x) = \sum_{i=1}^{n} f_i \prod_{k=0,k\neq i}^{n} \frac{x - x_k}{x_i - x_k}$$

Lagrange插值程序

```
function v=lagrange(x,y,u)
n=length(x);
v=zero(size(u));
for k=1:n
w=ones(size(u));
    for j=[1:k-1 k+1:n]
    w=(u-x(i))./(x(k)-x(j)).*w;
    end
v=v+w*y(k);
end
```

其中，x为插值点；y为插值；u为计算序列点；v为计算序列点值。

例子:

x	0.0	1.0	2.0	3.0
y	-5.0	-6.0	-1.0	16

样条函数插值(Spline interpolation)

$$p_i(x) = y_i + \frac{y_{i+1} - y_i}{x_{i+1} - x_i}(x - x_i)$$

$$s(x) = p_i(x), x_i \leq x < x_{i+1}$$

The most important case is the cubic spline which is given in the interval $x_i \leq x < x_{i+1}$ by

$$p_i(x) = \alpha_i + \beta_i(x - x_i) + \gamma_i(x - x_i)^2 + \delta_i(x - x_i)^3$$

If we hope to get smooth curve and assume that the interpolating function and their first tow derivatives are continuous, we have for the inner boundaryies

$$\begin{aligned} p_i(x_{i+1}) &= p_{i+1}(x_{i+1}), \\ p_i'(x_{i+1}) &= p_{i+1}'(x_{i+1}), \\ p_i''(x_{i+1}) &= p_{i+1}''(x_{i+1}). \end{aligned}$$

Continued

$$P_i''(x) = a_i x + b, x \in [x_i, x_{i+1}]$$

$$\begin{aligned} a_i x_i + b_i &= P_i''(x) = y_i'' \\ a_i x_{i+1} + b_i &= P_i''(x_{i+1}) = y_{i+1}'' \end{aligned}$$

$$a_i = \frac{y_{i+1}'' - y_i''}{x_{i+1} - x_i}, \ b_i = \frac{x_{i+1} y_i'' - x_i y_{i+1}''}{x_{i+1} - x_i}$$

where y_i'' and y_{i+1}'' are unkonwn. But we can use

$$\begin{aligned} S_i'(x) &= \frac{1}{2} a_i x^2 + b_i x + c_i \\ S_i(x) &= \frac{1}{6} a_i x^3 + \frac{1}{2} b_i x^2 + c_i x + d_i \end{aligned}$$

The coefficient c_i and d_i

$$\begin{aligned} c_i &= \frac{1}{6(x_{i+1}-x_i)}[(x_i^2-2x_{i+1}^2-2x_ix_{i+1})y_i''] \\ &+(2x_i^2-x_{i+1}^2+2x_ix_{i+1})y_{i+1}''+6(y_{i+1}-y_i)] \end{aligned}$$

$$\begin{aligned} d_i &= \frac{1}{6(x_{i+1}-x_i)}[(x_ix_{i+1}(-2x_{i+1}+x_i)y_i''] \\ &+x_ix_{i+1}(2x_i-x_{i+1})y_{i+1}''+6(x_iy_{i+1}-x_{i+1}y_i)] \end{aligned}$$

There exists n unknown parameters $y_i''(i=1,2,\cdots,n)$ in $\{S_i(x), i=1,2,\cdots,n-1\}$. 根据一阶导数的连续性有关系，

$$S_{i-1}'(x_i)=S_i'(x_i)$$

$i.e.$

$$\frac{1}{2}a_{i-1}x_i^2+b_{i-1}x_i+c_{i-1}=\frac{1}{2}a_ix_i^2+b_ix_i+c_i$$

三对角矩阵

把含有未知量$y''_i(i=1,2,\cdots,n)$的系数$a_i,b_i,c_i,a_{i-1},c_{i-1}$代入上式，得

$$\alpha_{i-1}y''_{i-1}+\beta_i y''_i+\gamma_i y''_{i=1}=f_i$$

$$\alpha_{i-1}=x_i-x_{i-1},\beta_i=2(x_{i+1}-x_{i-1}),\gamma_i=x_{i+1}-x_i$$

$$f_i=6(\frac{y_{i+1}-y_i}{\gamma_i}-\frac{y_i-y_{i-1}}{\alpha_{i-1}}),i=2,\cdots,n-1$$

是一个系数为三对角矩阵的代数方程。

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

再结合两个条件以决定n个未知量y_i'' $(i = 1, 2, \cdots, n)$,通常采用

1. 根据两端点的一阶导数，获得y''联立三对角矩阵构建线性代数方程组；
2. 设两端点的二阶导数为0。

利用三次样条插值。可求出差值曲线的一阶和二阶导数插值函数.

Examples:

对于函数$y = \frac{1}{1+x^2}$在区间[-1,1]求出三次样条插值函数。

1 插值法

2 拟合法
- 最小二乘法
- 线性拟合
- 多项式拟合

3 作业

The definition of fitting method

Fitting functions to data points，Most commonly, one fits a function of the form

$$y = f(x)$$

特点：

1. 拟合函数不必通过所有已知点(x_i,y_i),拟合的曲线能反映给定数据的整体趋势,并使拟合数据与已知节点的误差最小；
2. 拟合方法给出了一组分立数据的整体性质；
3. 函数通常可以反映一定的物理含义；

For instance, fitting lines and polynomial functions to data points

$$p(x) = p_m(x) = \sum_{j=1}^{m+1} a_j x^{j-1}, m < n$$

The least squares fitting is often used, namely

$$q(a_1, a_2, , \cdots, a_{m+1}) = \sum_{i=1}^{n} [p(x_i) - y_i]^2$$

For the given data (x_i,y_i) $(i = 1, 2, \cdots, n)$, they satisfy the following equation,

$$p(x) = a + bx$$

According to the least squares method, how to find the fitting parameters a and b make the all data points above satisfy the following equation

$$q(a, b) = \sum_{i=1}^{n} [(a + bx_i) - y_i]^2$$

and $q(a, b)$ have local minimum.

Continued

为使$q(a,b)$极小，a, b 必须满足下列方程组：

$$\begin{cases} \frac{\partial q}{\partial a} & = & 2\sum_{i=1}^{n}[(a+bx_i)-y_i] & = & 0 \\ \frac{\partial q}{\partial b} & = & 2\sum_{i=1}^{n}[(a+bx_i)-y_i]x_i & = & 0 \end{cases}$$

we can get

$$\begin{cases} a & = & \frac{n\sum y_i - \sum x_i^2 - \sum x_i \sum x_i y_i}{n\sum x_i^2 - (\sum x_i)^2} \\ b & = & \frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x_i^2 - (\sum x_i)^2} \end{cases}$$

The code for matlab

```
linearfit.m
function [a b]=linearfit (x,y)
n=length(x);
x2=x.*x; xy=x.*y;
sx=sum(x);   sy=sum(y);
sxy=sum(xy); sx2=sum(x2);
deno=n*sx2-sx*sx;
a=(sy*sx2-sx*sxy)/deno;
b=(n*sxy-sx*sy)/deno;
end
```

For m-order polynomial fitting,

$$p_m(x) = \sum_{j=1}^{m+1} a_j x^{j-1}, m < n$$

then the sum of squares for Error

$$Q(a_1, a_2, \cdots, a_{m+1}) = \sum_{i=1}^{n}(\sum_{j=1}^{m+1} a_j x_i^{j-1} - y_i)^2$$

Partial derivatives

$$\frac{\partial Q}{\partial a_k} = 2\sum_{i=1}^{n}(\sum_{j=1}^{m+1} a_j x_i^{j-1} - y_i)x_i^{k-1} = 0,$$

$k = 1, 2, \cdots, m+1$; or

$$\sum_{i=1}^{n} y_i x_i^{k-1} = \sum_{j=1}^{m+1} a_j \sum_{i=1}^{n} x_i^{j+k-2}$$

we define

$$S_k = \sum_{i=1}^{n} x_i^{k-1}, \quad T_k = \sum_{i=1}^{n} y_i x_i^{k-1}$$

$$\sum_{j=1}^{m+1} a_j S_{j+k-1} = T_k, k = 1, 2, \cdots, m+1$$

Code for the matlab

multifit.m

```
function a=multifit(x,y,m)
n=length(x);
c(1:(2*m+1))=0; T(1:(m+1))=0;
for j=1:(2*m+1)
for k=1:n
c(j)=c(j)+x(k)^(j-1)
if (j < (m+2))
T(j)=T(j)+y(k)*x(k)^(j-1);
end; end; end
S(1,:)=c(1: (m+1));
for k=2:(m+1)
S(k,:)=c(k:(m+k));
end
a=S / T';
```

作业

1. 利用二次插值计算(1) f(0.472); (2) f(x)=0.5, x=?, 所依据的数据表为

x	0.46	0.47	0.48	0.49	$\cdots$
$f(x)$	0.4846555	0.4937452	0.5027498	0.5116683	$\cdots$

2. 区间[0,2]上的三次样条插值函数

$$s(x) = \begin{cases} 2x^3 & 0 \le x \le 1 \\ x^3 + ax^2 + bx + c & 1 \le x \le 2 \end{cases}$$

求a, b, c.

3. 已知函数数据表

x_i	1	2	3	4	6	7	8
y_i	2	3	6	7	5	3	2

试用最小二乘法拟合二次多项式.

建议大家熟悉下列matlab中关于插值和拟合的函数命令：

1. interp1(x0,y0,x,'method');可实现一维情况下的x的插值y,方法有线性，三次样条等；interp2, interp3, meshgrid, etc.
2. P=polyfit(x0,y0,n), 通过基于最小二乘法的方法，可找拟合(x0,y0)的n次多项式的系数； [P,S]=polyfit(x0,y0,N): returns the polynomial coefficients P and a stracture S for use with POLYVAL to obtain error estimates for predictions.
3. 另了解lsqcurvefit， fminunc, nlinfit函数的使用。