现代数值计算方法

第四章 插值法与最小二乘拟合











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第四章 插值法与最小二乘拟合

§4.4 最小二乘法

§4.4.3 正交最小二乘拟合

最常见的拟合函数类是多项式,其基函数一般取幂函数

$$\varphi_0(x) = 1, \ \varphi_1(x) = x, \ \cdots, \varphi_m(x) = x^m.$$

由于

$$(\varphi_j, \varphi_k) = \sum_{i=1}^n x_i^{j+k}, \quad (f, \varphi_k) = \sum_{i=1}^n x_i^k y_i,$$













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这样, 法方程组为

$$\begin{pmatrix}
 n & \sum_{i=1}^{n} x_{i} & \cdots & \sum_{i=1}^{n} x_{i}^{m} \\
 \sum_{i=1}^{n} x_{i} & \sum_{i=1}^{n} x_{i}^{2} & \cdots & \sum_{i=1}^{n} x_{i}^{m+1} \\
 \vdots & \vdots & \cdots & \vdots \\
 \sum_{i=1}^{n} x_{i}^{m} & \sum_{i=1}^{n} x_{i}^{m+1} & \cdots & \sum_{i=1}^{n} x_{i}^{2m}
 \end{pmatrix}
\begin{pmatrix}
 a_{0} \\
 a_{1} \\
 \vdots \\
 a_{m}
 \end{pmatrix} = \begin{pmatrix}
 \sum_{i=1}^{n} y_{i} \\
 \sum_{i=1}^{n} x_{i} y_{i} \\
 \vdots \\
 \sum_{i=1}^{n} x_{i}^{m} y_{i}
 \end{pmatrix}.$$

$$(4.39)$$

但遗憾的是, 当 m 比较大时, 该方程组往往是病态的, 从而导致结果误差很大.

下面我们考虑所谓的正交最小二乘拟合. 首先给出正交多项式的概念.

定义 4.2 设节点 x_1, x_2, \dots, x_n 和多项式函数 P(x) 和 Q(x), 如













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果

$$(P,Q) = \sum_{i=1}^{n} P(x_i)Q(x_i) = 0,$$

则称 P(x) 和 Q(x) 关于节点 x_1, x_2, \dots, x_n 正交. 如果函数类 Φ 的基函数 $\psi_0, \psi_1, \dots, \psi_m$ 两两正交, 则称为一组正交基.

设 $\psi_0, \psi_1, \dots, \psi_m$ 为函数类 Φ 的一组正交基, 那么法方程组 (??) 就成为简单的对角方程组, 其解可以由下式直接给出:

$$a_k = \frac{(f, \psi_k)}{(\psi_k, \psi_k)}, \quad k = 0, 1, \dots, m,$$
 (4.40)

从而避免了求解病态方程组.

正交基可以由任意基 $\varphi_0, \varphi_1, \cdots, \varphi_m$ 通过 Schmit 正交化方法得到:













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$$\psi_0(x) = \varphi_0(x),$$

$$\psi_1(x) = \varphi_1(x)$$

$$\psi_1(x) = \varphi_1(x) - \frac{(\varphi_1, \psi_0)}{(\psi_0, \psi_0)} \psi_0(x),$$

$$\psi_2(x) = \varphi_2(x) - \frac{(\varphi_2, \psi_0)}{(\psi_0, \psi_0)} \psi_0(x) - \frac{(\varphi_2, \psi_1)}{(\psi_1, \psi_1)} \psi_1(x),$$
.....

$$\psi_m(x) = \varphi_m(x) - \frac{(\varphi_m, \psi_0)}{(\psi_0, \psi_0)} \psi_0(x) - \frac{(\varphi_m, \psi_1)}{(\psi_1, \psi_1)} \psi_1(x) - \cdots - \frac{(\varphi_m, \psi_{m-1})}{(\psi_{m-1}, \psi_{m-1})} \psi_{m-1}(x).$$

例 4.12 已知下列数据求拟合曲线 $\varphi(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$.

x	-2	-1	0	1	2
f(x)	-1	-1	0	1	1















解 取 $\varphi_0(x) = 1$, $\varphi_1(x) = x$, $\varphi_2(x) = x^2$, $\varphi_3(x) = x^3$, 先进行 Schmit 正交化:

$$\psi_0(x) = \varphi_0(x) = 1,$$

$$\psi_1(x) = \varphi_1(x) - \frac{(\varphi_1, \psi_0)}{(\psi_0, \psi_0)} \psi_0(x) = x,$$

$$((\varphi_1, \psi_1), \dots, (\varphi_1, \psi_1),$$

$$\psi_2(x) = \varphi_2(x) - \frac{(\varphi_2, \psi_0)}{(\psi_0, \psi_0)} \psi_0(x) - \frac{(\varphi_2, \psi_1)}{(\psi_1, \psi_1)} \psi_1(x) = x^2 - 2,$$

$$\psi_3(x) = \varphi_3(x) - \frac{(\varphi_3, \psi_0)}{(\psi_0, \psi_0)} \psi_0(x) - \frac{(\varphi_3, \psi_1)}{(\psi_1, \psi_1)} \psi_1(x) - \frac{(\varphi_3, \psi_2)}{(\psi_2, \psi_2)} \psi_2(x)$$

$$= x^3 - \frac{17}{5}x.$$
则 $\psi_0, \psi_1, \psi_2, \psi_3$ 两两正交. 计算得
$$(\psi_0, \psi_0) = 5 \quad (\psi_1, \psi_1) = 10 \quad (\psi_2, \psi_2) = 14 \quad (\psi_2, \psi_2) = 14 4$$

 $(\psi_0, \psi_0) = 5, \quad (\psi_1, \psi_1) = 10, \quad (\psi_2, \psi_2) = 14, \quad (\psi_3, \psi_3) = 14.4,$ $(f, \psi_0) = 0, \quad (f, \psi_1) = 6, \quad (f, \psi_2) = 0, \quad (f, \psi_3) = -2.4.$

从而,由(4.40)得

$$a_0 = 0$$
, $a_1 = \frac{6}{10} = \frac{3}{5}$, $a_2 = 0$, $a_3 = \frac{-2.4}{14.4} = -\frac{1}{6}$.

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$$\varphi(x) = \frac{3}{5}\psi_1(x) - \frac{1}{6}\psi_3(x) = \frac{3}{5}x - \frac{1}{6}\left(x^3 - \frac{17}{5}x\right) = \frac{7}{6}x - \frac{1}{6}x^3.$$

§4.4.4 多项式拟合的通用程序

下面给出多项式拟合的 MATLAB 通用程序:

● 多项式拟合 MATLAB 程序

%mafit.m

故

function p=mafit(x,y,m)

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```
%用途:多项式拟合
%格式: p=mafit(x,y,m) x,y为数据向量, m为拟合
      多项式次数,p返回多项式系数降幂排列
format short;
A=zeros(m+1,m+1);
for i=0:m
  for j=0:m
     A(i+1,j+1) = sum(x.^{(i+j)});
  end
  b(i+1) = sum(x.^i.*y);
end
a=A\b';
p=fliplr(a'); %按降幂排列
```

例 4.13 用上述程序求解例 4.12.

解 在 MATLAB 命令窗口执行

得计算结果:

-0.1667 0 1.1667

从而所求的拟合曲线为

$$\varphi(x) = -0.1667x^3 + 1.1667x.$$

作业: P92: 4.25; 4.28.

















