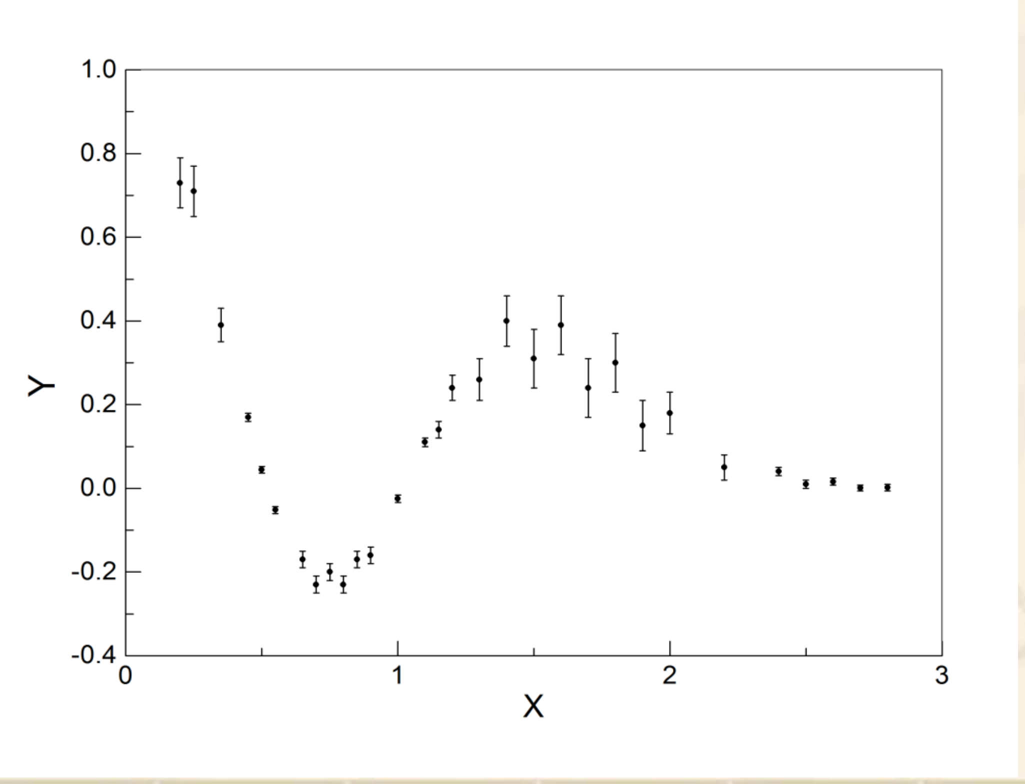
练习：非线性最佳平方拟合

一、数据点 $\{x_i, y_i, \pm\Delta y_i\}_{i=0}^{N}$

{0.20,0.73,0.06},{0.25,0.71,0.06},{0.35,0.39,0.04},{0.45,0.17,0.01},{0.50,0.044,0.008},
{0.55,-0.052,0.008},{0.65,-0.17,0.02},{0.70,-0.23,0.02},{0.75,-0.20,0.02},{0.80,-0.23,0.02},
{0.85,-0.17,0.02},{0.90,-0.16,0.02},{1.00,-0.025,0.009},{1.10,0.11,0.01},{1.15,0.14,0.02},
{1.20,0.24,0.03},{1.30,0.26,0.05},{1.40,0.40,0.06},{1.50,0.31,0.07},{1.60,0.39,0.07},
{1.70,0.24,0.07},{1.80,0.30,0.07},{1.90,0.15,0.06},{2.00,0.18,0.05},{2.20,0.05,0.03},
{2.40,0.04,0.01},{2.50,0.01,0.01},{2.60,0.016,0.008},{2.70,0.001,0.007},{2.80,0.002,0.008}



二、拟合函数（非线性的）：

$$P(x) = \left(1 + a_1 \cdot x + a_2 \cdot x^2\right) \exp\left(-a_3 \cdot x^2\right)$$

参量范围：$-6 \le a_1 \le 6,\ 0 \le a_2 \le 6,\ 0 \le a_3 \le 5$

三、非线性最佳平方拟合：搜索得到 $a_1^*,\ a_2^*,\ a_3^*$

使得 $Q(a_1, a_2, a_3) = \sum_{i=0}^{n} \frac{1}{\sigma_i^2} \left[y_i - P(x_i, a_1, a_2, a_3)\right]^2$ 最小

四、梯度搜索法：

任意取初值：$\left\{a_1^{(0)} \in (-6, 6),\ a_2^{(0)} \in (0, 6),\ a_3^{(0)} \in (0, 5)\right\}$

适当取增量：$\left\{\Delta a_1 \sim 0.02,\ \Delta a_2 \sim 0.02,\ \Delta a_3 \sim 0.02\right\}$

计算：$\frac{\partial Q}{\partial a_1} = \frac{Q(a_1^{(0)} + \Delta a_1, a_2^{(0)}, a_3^{(0)}) - Q(a_1^{(0)}, a_2^{(0)}, a_3^{(0)})}{\Delta a_1},\quad \frac{\partial Q}{\partial a_2} = \ ,\quad \frac{\partial Q}{\partial a_3} =$

计算：$\chi_1 = \frac{\partial Q}{\partial a_1} / \sqrt{\left(\frac{\partial Q}{\partial a_1}\right)^2 + \left(\frac{\partial Q}{\partial a_1}\right)^2 + \left(\frac{\partial Q}{\partial a_3}\right)^2}$， $\chi_2 =$ ，$\chi_3 =$

$$\delta a_1 = -\Delta a_1 \chi_1,\ \delta a_2 = -\Delta a_2 \chi_2,\ \delta a_3 = -\Delta a_3 \chi_3$$

$$a_1^{(1)} = a_1^{(0)} + \delta a_1,\ a_2^{(1)} = a_2^{(0)} + \delta a_2,\ a_3^{(1)} = a_3^{(0)} + \delta a_3$$

计算得出搜索点的： $Q^{(1)}(a_1^{(1)}, a_2^{(1)}, a_3^{(1)})$

判断比较：$Q^{(1)}(a_1^{(1)}, a_2^{(1)}, a_3^{(1)}) < Q^{(0)}(a_1^{(0)}, a_2^{(0)}, a_3^{(0)})$

不满足, 调节各参数初值或增量： $\left\{a_j^{(0)} = \cdots, \Delta a_j = \cdots\right\}_{j=1}^{M}$

满足, 循环上面步骤直到：

$$Q^{(0)}(a_1^0, a_2^0) > Q^{(1)}(a_1^1, a_2^1) > Q^{(2)}(a_1^2, a_2^2) > \cdots > Q^{(*)}(a_1^*, a_2^*)$$

编程计算要点

一、输入模块（文档）

1、数据点 $\{\, x_i,\ y_i,\ \pm\Delta y_i\}_{i=0}^{N}$

2、参量（范围、初值、增量）$\{al_j,\ au_j,\ a_j^{(0)},\ \Delta a_j\}_{j=1}^{M}$

二、拟合函数模块（子程序）： $P(x,a)$ （参数组 $a[1:M]$）

三、均方差模块（子程序）： $Q(a)=\sum_{i=0}^{N}\frac{1}{(\Delta y_i)^2}[y_i-P(x_i,a)]^2$

四、梯度搜索法模块（子程序）： $GRAD(a,\cdots)$

1、由 $\{\, a_j\}_{j=1}^{M} \Rightarrow Q(a)$

2、由 $\{\, a_j\}_{j=1}^{M} \Rightarrow \{\, a_j+\delta a_j\}_{j=1}^{M} \Rightarrow Q(a+\delta a)$

注： $\delta a_j=-\Delta a_j\chi_j,\ \chi_j=\frac{\partial Q}{\partial a_j}\Big/\sqrt{\sum_i^M\left(\frac{\partial Q}{\partial a_i}\right)^2},\ \frac{\partial Q}{\partial a_j}=\frac{Q(a+\Delta a_j)-Q(a)}{\Delta a_j}$

3、判断比较： $Q(a+\delta a) < Q(a)$

满足：赋值 $\{ a_j \}_{j=1}^{M} = \{ a_j + \delta a_j \}_{j=1}^{M}$ ，循环执行 2、3

不满足：(1) 还原 $\{ a_j \}_{j=1}^{M}$ 调改增量 $\{ \delta a_j = \delta a_j / 2 \}_{j=1}^{M}$ ，回到执行 2

(2) 重新赋初值 $\{ a_j =, \cdots \}_{j=1}^{M}$ ，返回执行 1

注：避免无限循环计算，每计算一次 $NM = NM + 1$

当： $NM \geq N_{\max}$ 跳出循环计算

4、输出最后一次计算的结果：$Q^{(*)}(a^*)$, $\{ a_j^* \}_{j=1}^{M}$

五、检查拟合结果

1、作出拟合结果 $P(x, a^*)$ 曲线与实验数据比较图

2、考察取不同的参量初值和增量 $\{ a_j^{(0)}, \Delta a_j \}_{j=1}^{M}$ 的拟合结果