第 4 章实验建模

韩建伟

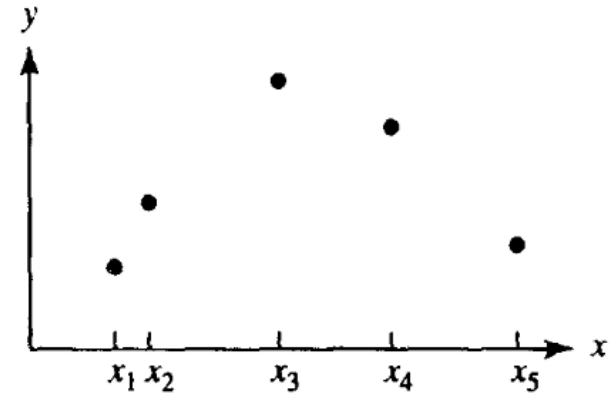
信息学院
mm@hanjianwei.com

2017/11/03

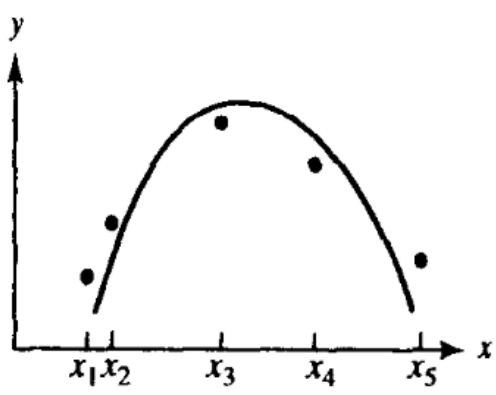
拟合和插值的选择

拟合 建模者利用一些假定来选择一个特定的模型类型，以解释观测值反应的状况.

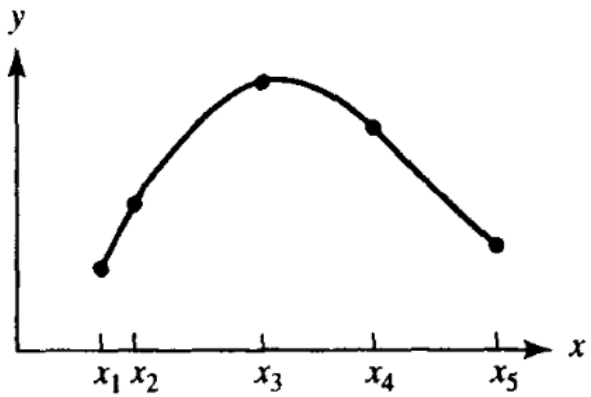
插值 建模者不可能构造一个满意地解释已知状况的易于处理的模型.



(a) 数据



(b) 拟合

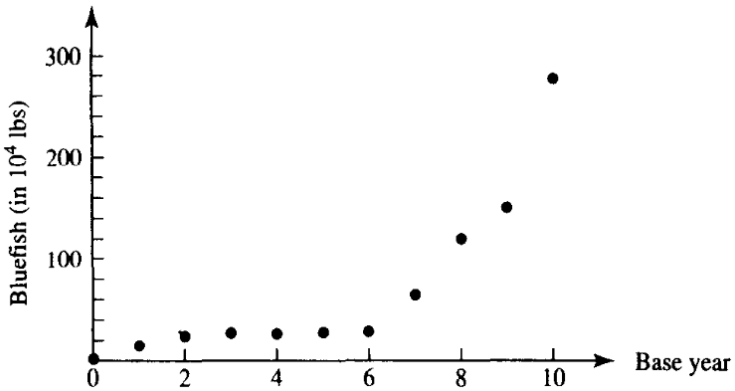


(c) 插值

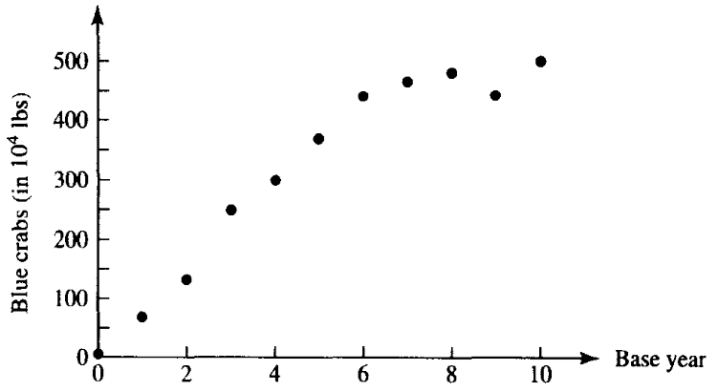
Chesapeake 海湾的收成

Year	Bluefish (lbs)	Blue crabs (lbs)
1940	15,000	100,000
1945	150,000	850,000
1950	250,000	1,330,000
1955	275,000	2,500,000
1960	270,000	3,000,000
1965	280,000	3,700,000
1970	290,000	4,400,000
1975	650,000	4,660,000
1980	1,200,000	4,800,000
1985	1,500,000	4,420,000
1990	2,750,000	5,000,000

(a) 收成数据



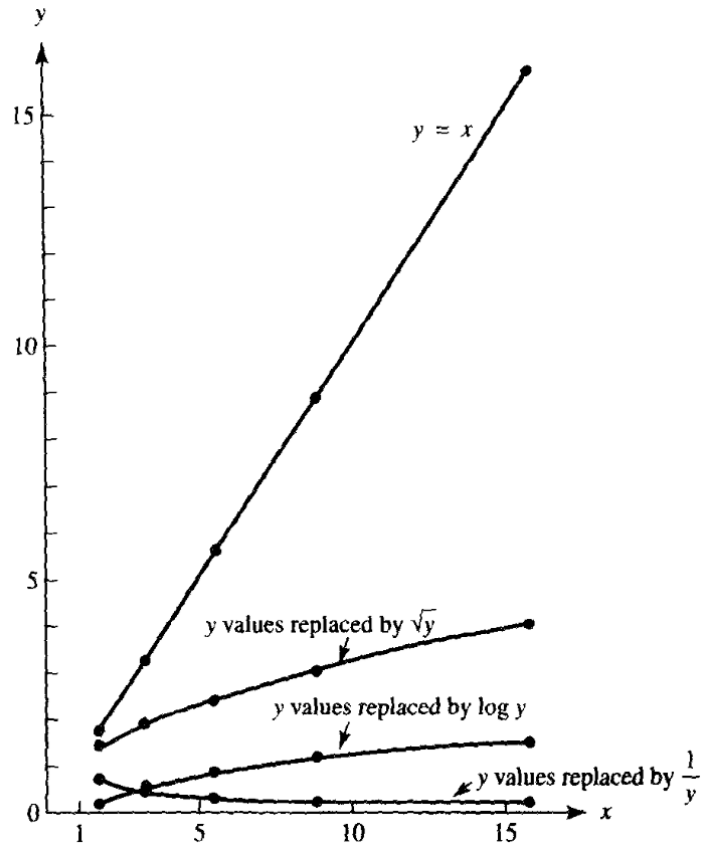
(b) 蓝鱼散点图



(c) 蓝蟹散点图

图: 1992 年《每日评论》收集的过去 50 年中 Chesapeake 海湾的海产收成.

如何对数据进行变换



(a) 三种变换

$$
\begin{array}{c}
\vdots \\
z^3 \\
z^2 \\
z \text{ (no change)} \\
* \left\{ \begin{array}{l} \sqrt{z} \\ \log z \\ \dfrac{-1}{\sqrt{z}} \\ \dfrac{-1}{z} \end{array} \right. \\
\dfrac{-1}{z^2} \\
\vdots
\end{array}
$$

*Most often used transformations

(b) 变换阶梯

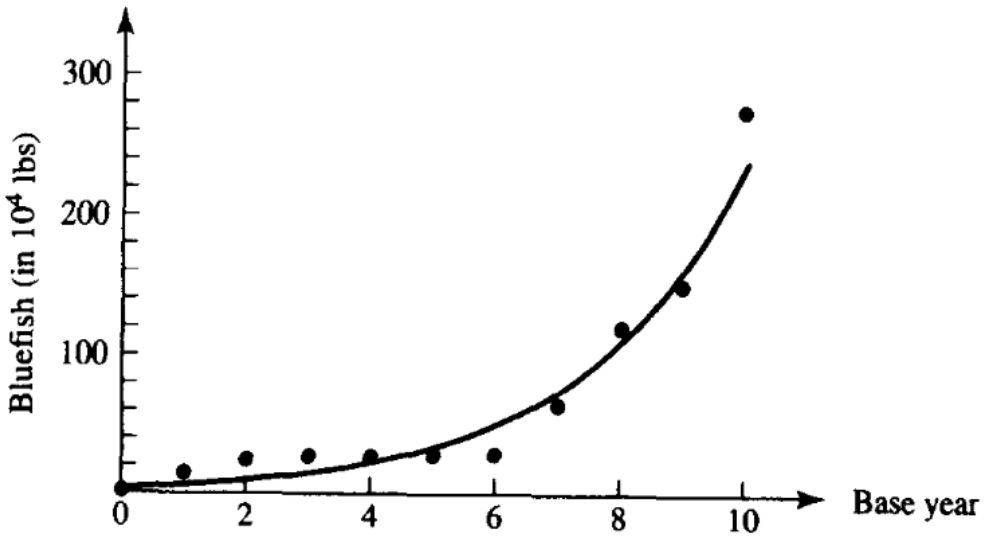
收获蓝鱼

- “向下压”曲线的右端，用最小二乘法拟合下列模型:

$$\log y = mx + b$$

Year	Base year	Bluefish (lbs)
	x	y
1940	0	15,000
1945	1	150,000
1950	2	250,000
1955	3	275,000
1960	4	270,000
1965	5	280,000
1970	6	290,000
1975	7	650,000
1980	8	1,200,000
1985	9	1,550,000
1990	10	2,750,000

(a) 蓝鱼数据



(b) 蓝鱼拟合 $y = 5.457(1.4635)^x$

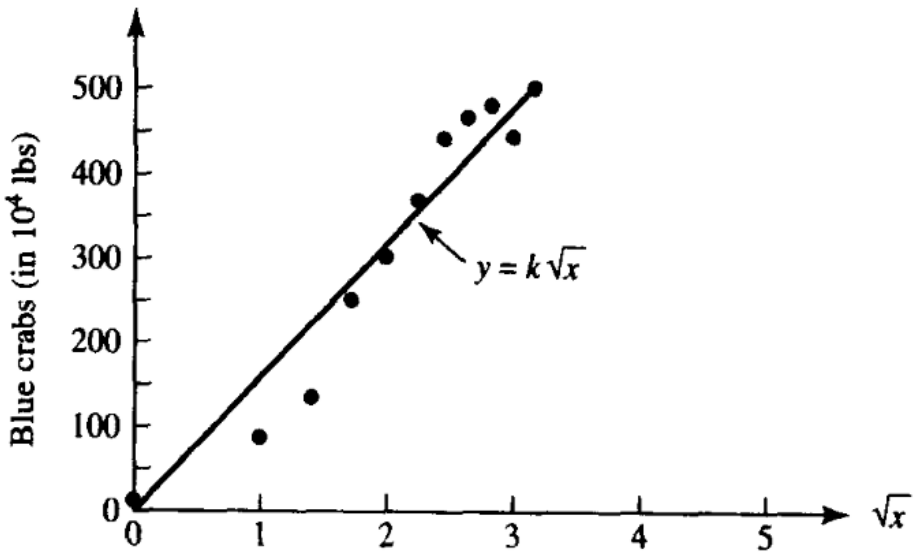
收获蓝蟹

- “向上扳”曲线的右端，用最小二乘法拟合下列模型：

$$y = k\sqrt{x}$$

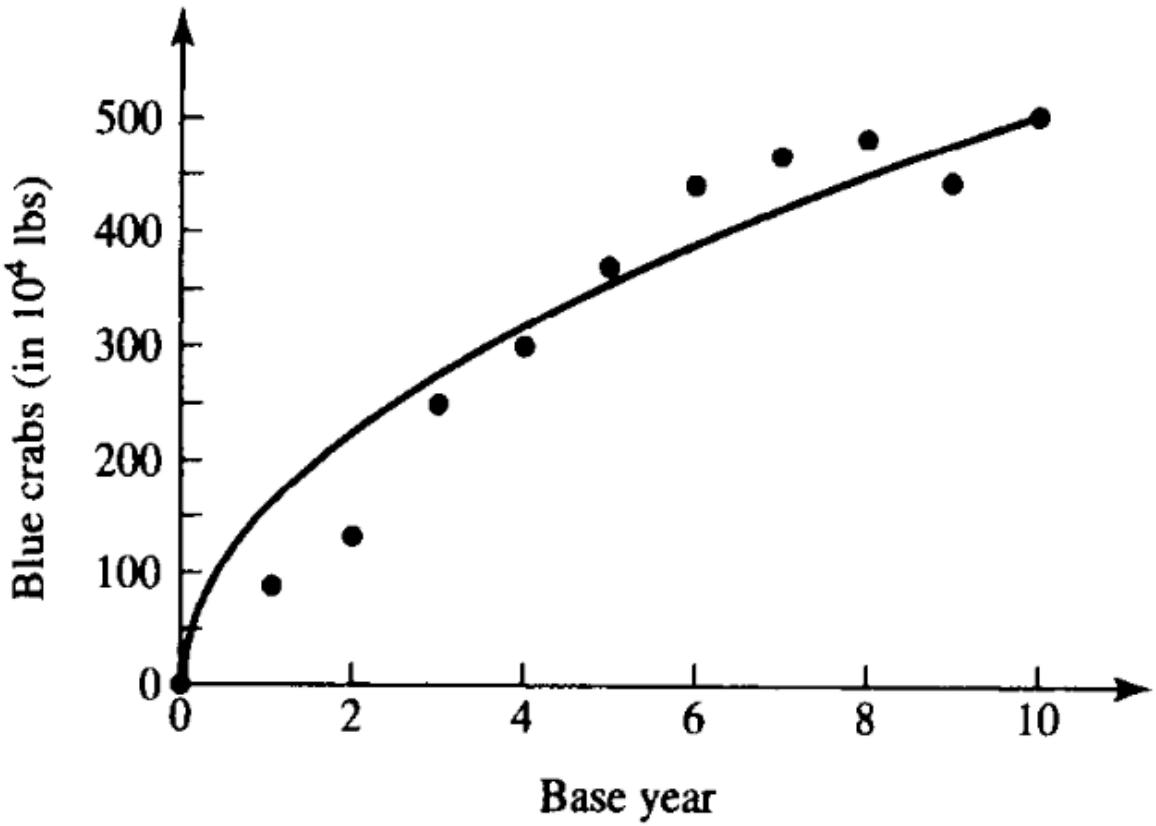
Year	Base year	Blue crabs (lbs)
	x	y
1940	0	100,000
1945	1	850,000
1950	2	1,330,000
1955	3	2,500,000
1960	4	3,000,000
1965	5	3,700,000
1970	6	4,400,000
1975	7	4,660,000
1980	8	4,800,000
1985	9	4,420,000
1990	10	5,000,000

(a) 蓝蟹数据



(b) 蓝蟹拟合直线 $y = 158.344\sqrt{x}$

蓝蟹最终拟合数据



验证模型

- 针对每一对数据，计算残差和相对误差.
- 对未来进行预测或者外推，这些模型是否依然适用.
- 这些简单的单项模型应该用于插值而不是外推.

本节的想法

构造一个模型时，从细心分析收集到的数据开始:

1. 看数据存在什么样的倾向
2. 是否有明显处于倾向以外的点？如果有这样的异常值，想想是否抛弃它们？如果是实验观测到的，重复该实验做一个数据收集错误的检查.
3. 当倾向确实清楚存在时，下一步是找到一个将数据变换成一（近似）直线的函数.
4. 警惕变换的使用如何带来欺骗性，特别是当数据点集中在一起时.
5. 最后，用第 3 章讨论的指示量分析拟合优度，记住对原始的而不是变换后的数据画出所提供的模型.
6. 如果对这一拟合不满意，可以研究其它的单项模型.

高阶多项式模型

- 单项模型易于进行模型分析，包括敏感性分析、优化、变化率以及曲线下面积的估计.
- 单项模型的可用性有限.
- 解决方案：多项模型.

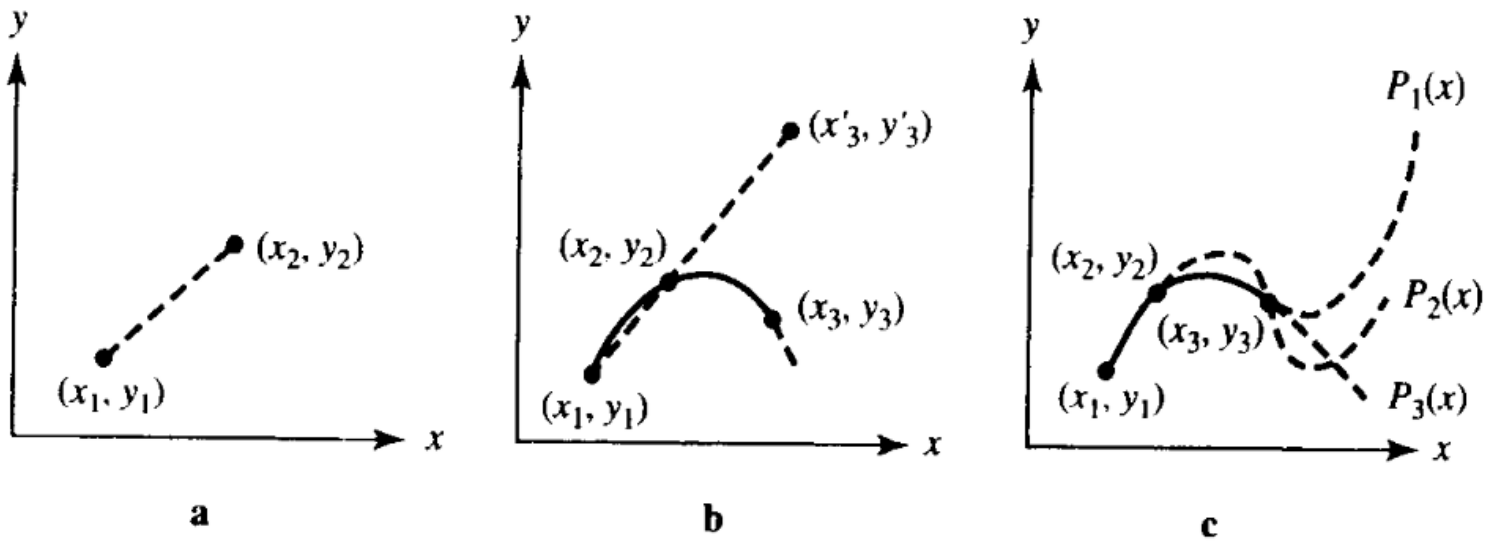


图: 通过三个数据点且最高阶为 2 的多项式只有唯一一个，而阶高于 2 的多项式有无穷多个

录音机的播放时间

c_i	100	200	300	400	500	600	700	800
t_i(sec)	205	430	677	945	1233	1542	1872	2224

图: 录音机计数器和播放时间关系表

我们有 8 个数据点，应期望一个最高阶为 7 的唯一多项式，记为

$$P_7(c) = a_0 + a_1 c + a_2 c^2 + a_3 c^3 + a_4 c^4 + a_5 c^5 + a_6 c^6 + a_7 c^7$$

把 8 个数据点代入

$$205 = a_0 + a_1 1 + a_2 1^2 + a_3 1^3 + a_4 1^4 + a_5 1^5 + a_6 1^6 + a_7 1^7$$

$$430 = a_0 + a_1 2 + a_2 2^2 + a_3 2^3 + a_4 2^4 + a_5 2^5 + a_6 2^6 + a_7 2^7$$

$$\vdots$$

$$2224 = a_0 + a_1 8 + a_2 8^2 + a_3 8^3 + a_4 8^4 + a_5 8^5 + a_6 8^6 + a_7 8^7$$

系数求解

$$
\begin{aligned}
a_0 &= -13.9999923 & a_4 &= -5.354166491 \\
a_1 &= 232.9119031 & a_5 &= 0.8013888621 \\
a_2 &= -29.08333188 & a_6 &= -0.0624999978 \\
a_3 &= 19.78472156 & a_7 &= 0.0019841269
\end{aligned}
$$

c_i	100	200	300	400	500	600	700	800
t_i	205	430	677	945	1233	1542	1872	2224
$P_7(c_i)$	205	430	677	945	1233	1542	1872	2224

考虑第 3 章提出的评判标准... 该模型真的是最好的吗?

多项式的拉格朗日形式

定理 1

如果 $x_0,x_1,...,x_n$ 是 $n+1$ 个不同的点，而 $y_0,y_1,...,y_n$ 是这些点上对应的观测值，那么，存在一个唯一的最高阶为 n 的多项式 $P(x)$，具有性质

$$y_k = P(x_k), k = 0, 1, ..., n$$

这一多项式由下式给定

$$P(x) = y_0 L_0(x) + ... + y_n L_n(x)$$

其中

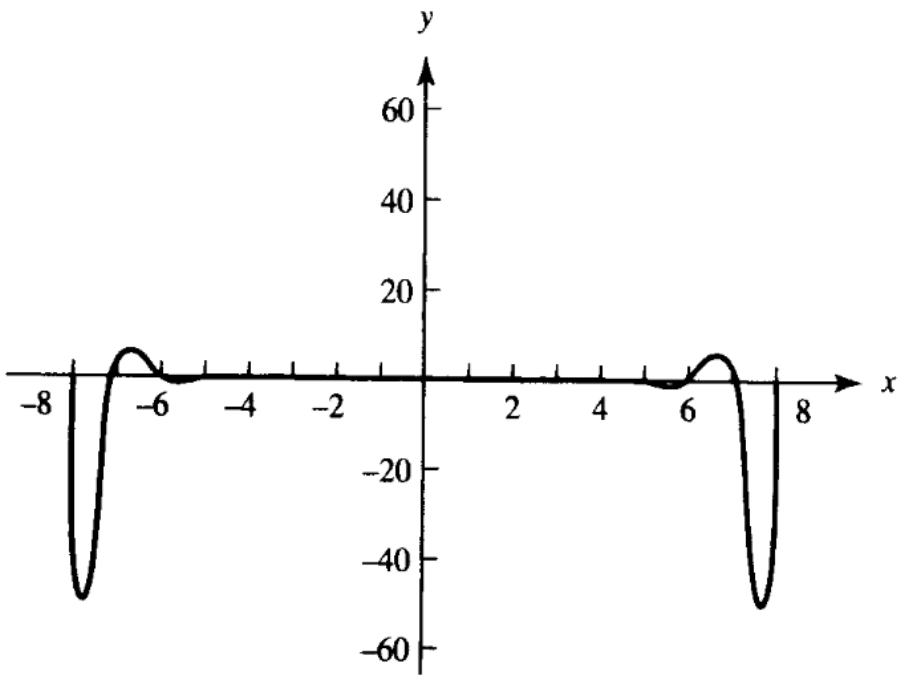
$$L_k(x) = \frac{(x-x_0)(x-x_1)...(x-x_{k-1})(x-x_{k+1})...(x-x_n)}{(x_k-x_0)(x_k-x_1)...(x_k-x_{k-1})(x_k-x_{k+1})...(x_k-x_n)}$$

高阶多项式的优缺点

缺点 1

在端点附近多项式有严重摆动, 进行数据预测时有很大问题

x_i	−8	−7	−6	−5	−4	−3	−2	−1	0	1	2	3	4	5	6	7	8
y_i	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

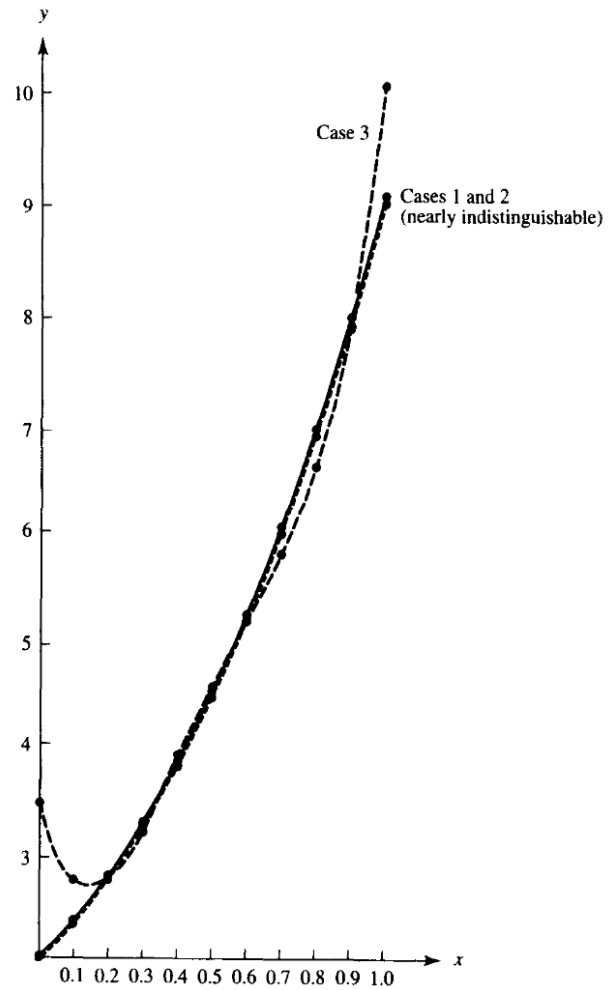


高阶多项式的优缺点

缺点 2

对数据微小变换非常敏感

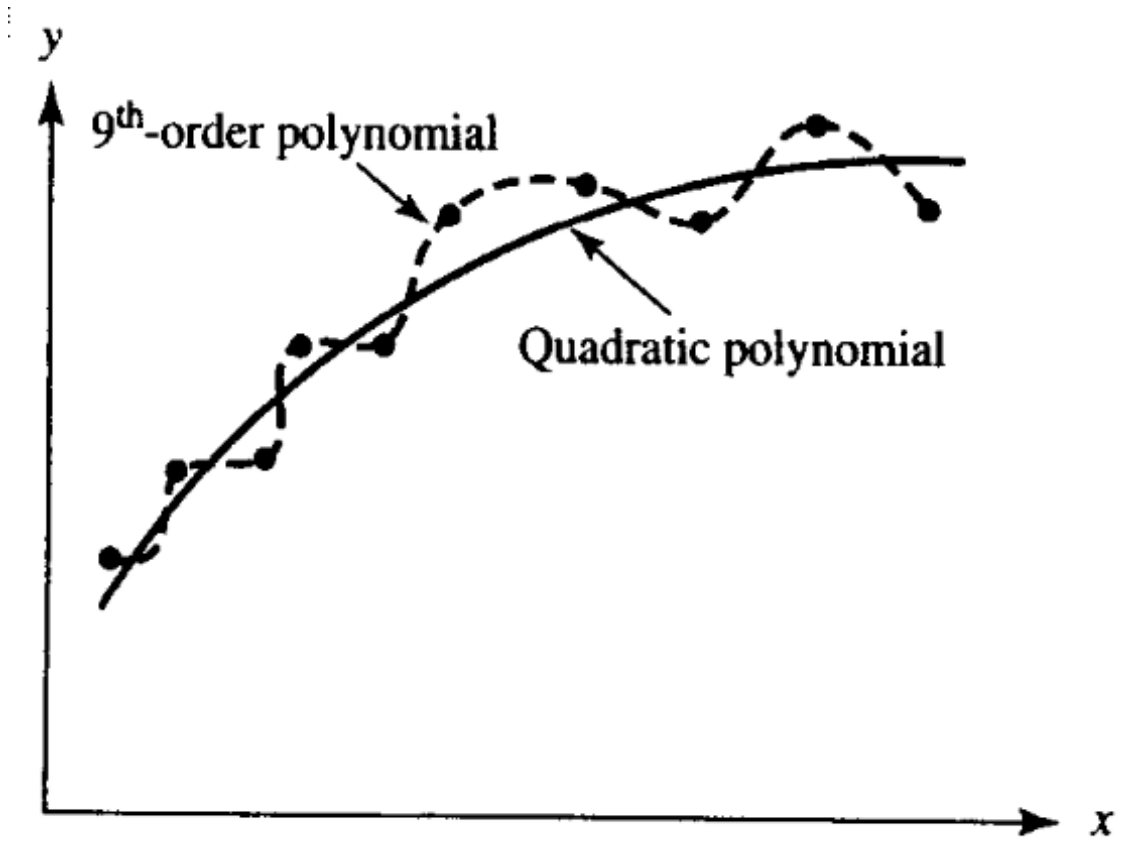
x_i	0.2	0.3	0.4	0.6	0.9
Case 1: y_i	2.7536	3.2411	3.8016	5.1536	7.8671
Case 2: y_i	2.754	3.241	3.802	5.154	7.867
Case 3: y_i	2.7536	3.2411	3.8916	5.1536	7.8671



光滑化：低阶多项式模型

光滑化

不管数据的个数, 选取一个低阶多项式，通过第 3 章的准则拟合给定的数据.



再论录音机的播放时间

c_i	100	200	300	400	500	600	700	800
t_i (sec)	205	430	677	945	1233	1542	1872	2224

图: 录音机计数器和播放时间关系表

拟合一个下列形式的二阶多项式

$$P_2(c) = a + bc + dc^2$$

用最小二乘法确定 $a,\ b,\ c$.

最小二乘法拟合

$$\text{Minimize } S = \sum_{i=1}^{m} [t_i - (a + bc_i + dc_i^2)]^2$$

存在极小点的必要条件

$$\frac{\partial S}{\partial a} = \frac{\partial S}{\partial b} = \frac{\partial S}{\partial d} = 0$$

故

$$ma + (\sum c_i)b + (\sum c_i^2)d = \sum t_i$$

$$(\sum c_i)a + (\sum c_i^2)b + (\sum c_i^3)d = \sum c_i t_i$$

$$(\sum c_i^2)a + (\sum c_i^3)b + (\sum c_i^4)d = \sum c_i^2 t_i$$

拟合结果

$$P_2(c) = 0.14286 + 1.94226c + 0.00105c^2$$

c_i	100	200	300	400	500	600	700	800
t_i	205	430	677	945	1233	1542	1872	2224
$t_i - P_2(c_i)$	0.167	−0.452	0.000	0.524	0.119	−0.214	−0.476	0.333

1. 应该用一个多项式吗?
2. 如果应该，几阶的多项式合适?

多项式阶数的确定

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

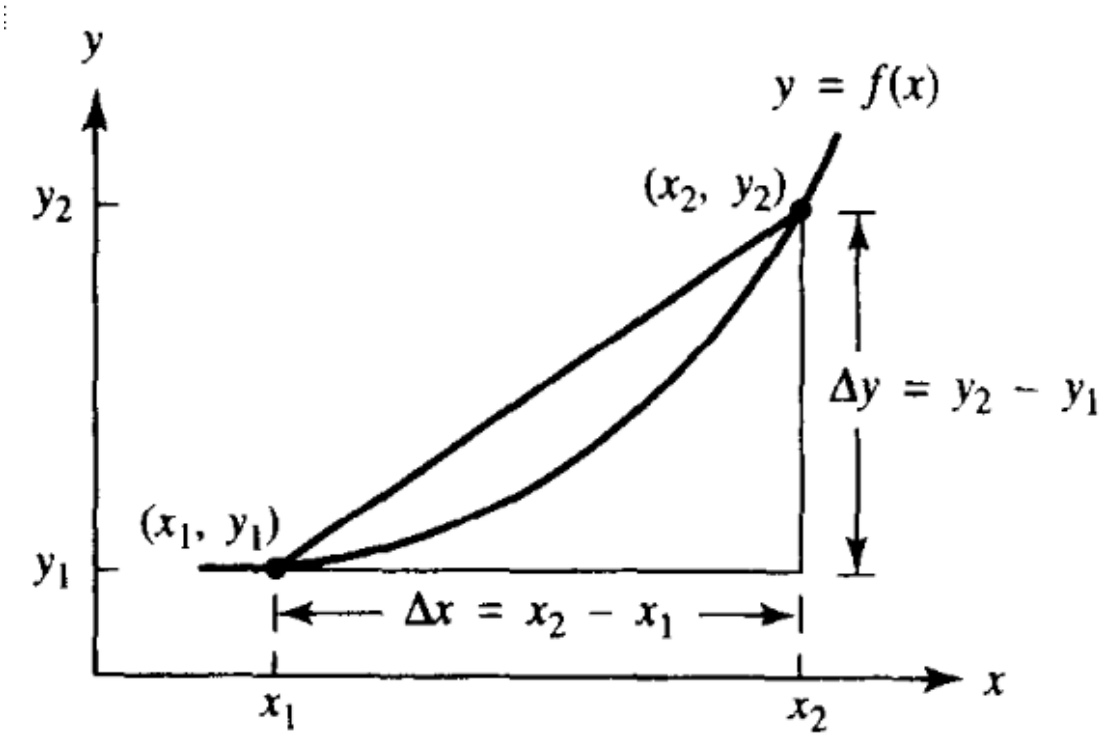
$$P'(x) = b + 2cx$$

$$P''(x) = 2c$$

$$P'''(x) = 0$$

导数的离散形式

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x}$$



离散求导示例

Data		Differences			
x_i	y_i	Δ	Δ^2	Δ^3	Δ^4
0	0				
		4			
2	4		8		
		12		0	
4	16		8		0
		20		0	
6	36		8		
		28			
8	64				

Data		First divided difference	Second divided difference
x_1	y_1		
		$\frac{y_2 - y_1}{x_2 - x_1}$	
x_2	y_2		$\frac{\frac{y_3 - y_2}{x_3 - x_2} - \frac{y_2 - y_1}{x_2 - x_1}}{x_3 - x_1}$
		$\frac{y_3 - y_2}{x_3 - x_2}$	
x_3	y_3		

图: 一阶、二阶导数的离散计算

再论录音机的播放时间

Data		Divided differences			
x_i	y_i	Δ	Δ^2	Δ^3	Δ^4
100	205				
		2.2500			
200	430		0.0011		
		2.4700		0.0000	
300	677		0.0011		0.0000
		2.6800		0.0000	
400	945		0.0010		0.0000
		2.8800		0.0000	
500	1233		0.0011		0.0000
		3.0900		0.0000	
600	1542		0.0011		0.0000
		3.3000		0.0000	
700	1872		0.0011		
		3.5200			
800	2224				

图: 录音机数据的均差表

可以看到，二阶均为常数，三阶均差到小数点后 4 位均为 0，可以看出数据基本是二次的，可以用二次多项式作为经验模型.

差分表中的观测值

- 对“小”的评判是相对的、定性的.
- 必须灵敏地感觉数据中出现的误差和不规则变化.

车辆的停止距离

Speed v (mph)	20	25	30	35	40	45	50	55	60	65	70	75	80
Distance d (ft)	42	56	73.5	91.5	116	142.5	173	209.5	248	292.5	343	401	464

Data		Divided differences			
v_i	d_i	Δ	Δ^2	Δ^3	Δ^4
20	42				
		2.2800			
25	56		0.0700		
		3.5000		−0.0040	
30	73.5		0.0100		0.0006
		3.6000		0.0080	
35	91.5		0.1300		−0.0007
		4.9000		−0.0060	
40	116		0.0400		0.0004
		5.3000		0.0027	
45	142.5		0.0800		0.0000
		6.1000		0.0027	
50	173		0.1200		−0.0004
		7.3000		−0.0053	
55	209.5		0.0400		0.0005
		7.7000		0.0053	
60	248		0.1200		−0.0003
		8.9000		0.0000	
65	292.5		0.1200		0.0001
		10.1000		0.0020	
70	343		0.1500		−0.0003
		11.6000		−0.0033	
75	401		0.1000		
		12.6000			
80	464				

用二阶模型进行拟合

$$P(v) = a + bv + cv^2$$

用最小二乘法求解:

$$\text{Minimize } S = \sum_{i=1}^{m} [d_i - (a + bv_i + cv_i^2)]^2$$

存在极小点的必要条件 $\frac{\partial S}{\partial a} = \frac{\partial S}{\partial b} = \frac{\partial S}{\partial c} = 0$, 故

$$ma + (\sum v_i)b + (\sum v_i^2)c = \sum d_i$$

$$(\sum v_i)a + (\sum v_i^2)b + (\sum v_i^3)c = \sum v_i d_i$$

$$(\sum v_i^2)a + (\sum v_i^3)b + (\sum v_i^4)c = \sum v_i^2 d_i$$

模型验证

$$P(v) = 50.0594 - 1.9701v + 0.0886v^2$$

v_i	20	25	30	35	40	45	50
d_i	42	56	73.5	91.5	116	142.5	173
$d_i - P(v_i)$	−4.097	−0.182	2.804	1.859	2.985	1.680	−0.054

v_i	55	60	65	70	75	80
d_i	209.5	248	292.5	343	401	464
$d_i - P(v_i)$	−0.719	−2.813	−3.838	−3.292	0.323	4.509

图: 用二次多项式光滑化停止距离

当 $v = 0$ 时呢?

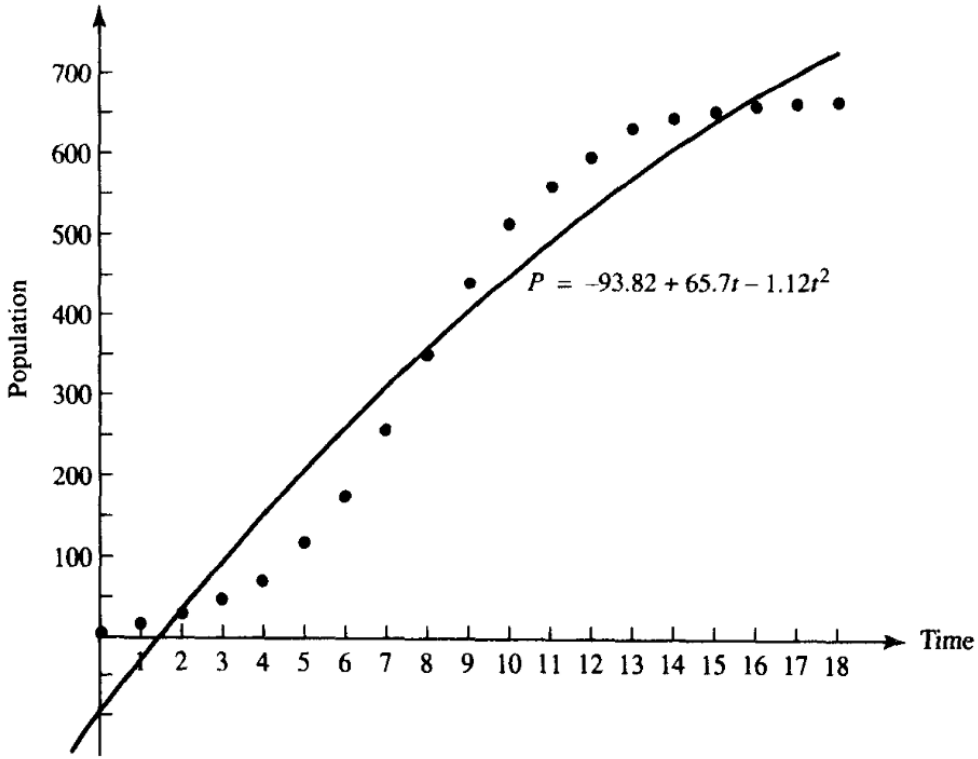
酵母培养物的增长

Data		Divided differences			
t_i	P_i	Δ	Δ^2	Δ^3	Δ^4
0	9.60				
		8.70			
1	18.30		1.00		
		10.70		0.92	
2	29.00		3.75		−0.31
		18.20		−0.30	
3	47.20		2.85		0.84
		23.90		3.07	
4	71.10		12.05		−1.46
		48.00		−2.77	
5	119.10		3.75		1.51
		55.50		3.28	
6	174.60		13.60		−1.51
		82.70		−2.75	
7	257.30		5.35		0.11
		93.40		−2.30	
8	350.70		−1.55		−0.05
		90.30		−2.48	
9	441.00		−9.00		0.29
		72.30		−1.32	
10	513.30		−12.95		0.94
		46.40		2.43	
11	559.70		−5.65		−0.16
		35.10		1.80	
12	594.80		−0.25		−1.40
		34.60		−3.78	
13	629.40		−11.60		1.87
		11.40		3.68	
14	640.80		−0.55		−1.10
		10.30		−0.73	
15	651.10		−2.75		0.37
		4.80		0.73	
16	655.90		−0.55		−0.20
		3.70		−0.07	
17	659.60		−0.75		
		2.20			
18	661.80				

图: 差分表

拟合结果

$$P = -93.82 + 65.70t - 1.12t^2$$



拟合失败!

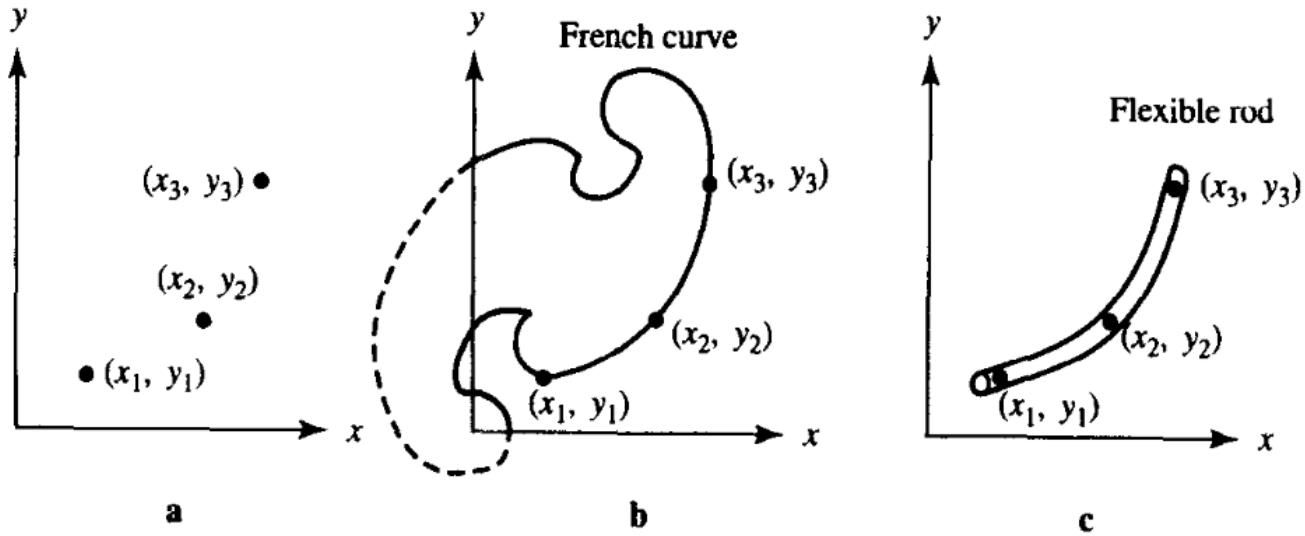
三阶样条模型

在连续的数据点对间使用不同的三阶多项式，追踪数据的趋势.

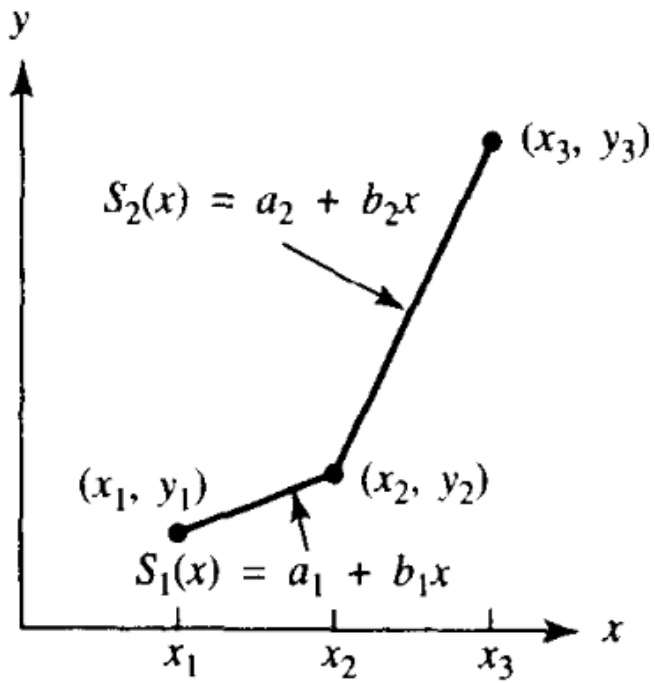
高阶多项式 端点处有摆动倾向，对数据中小的变化太敏感

低阶多项式 拟合效果不好（如速度很快时的刹车问题模拟）

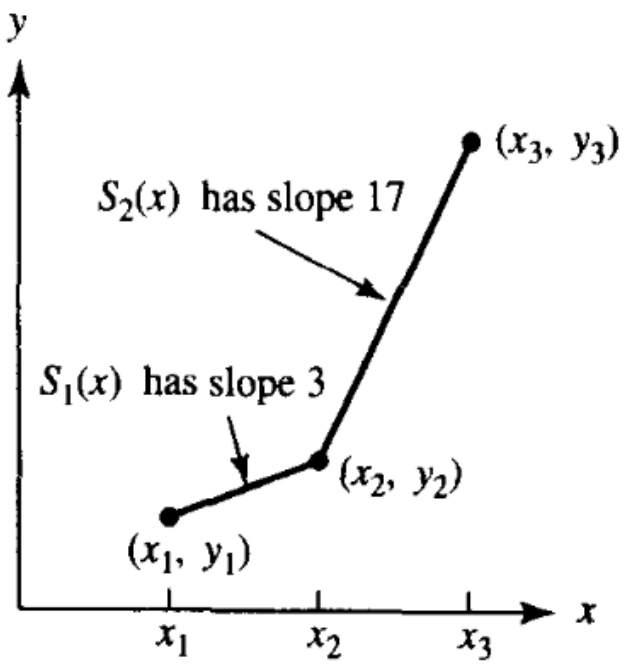
三阶样条插值 既保证基本关系的特征，同时减少摆动的倾向和数据变换的敏感性



线性样条

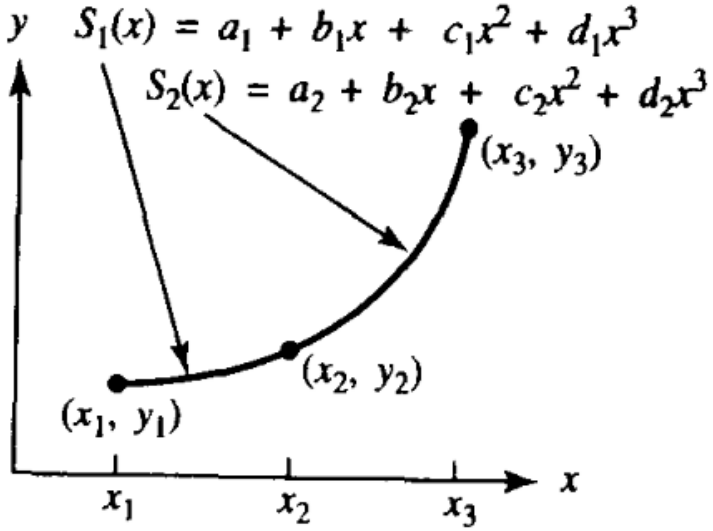


(a) 线性样条是含直线段的连续函数



(b) 由于一阶导数不连续，线性样条不光滑

三阶样条



$$S_1(x) = a_1 + b_1x + c_1x^2 + d_1x^3, x \in [x_1, x_2)$$

$$S_2(x) = a_2 + b_2x + c_2x^2 + d_2x^3, x \in [x_2, x_3)$$

三阶样条求解

$$S_1'(x) = b_1 + 2c_1x + 3d_1x^2, x \in [x_1, x_2)$$

$$S_1''(x) = 2c_1 + 6d_1x, x \in [x_1, x_2)$$

$$S_2'(x) = b_2 + 2c_2x + 3d_2x^2, x \in [x_2, x_3)$$

$$S_2''(x) = 2c_2 + 6d_2x, x \in [x_2, x_3)$$

求解:

$$S_1(x_1) = y_1$$

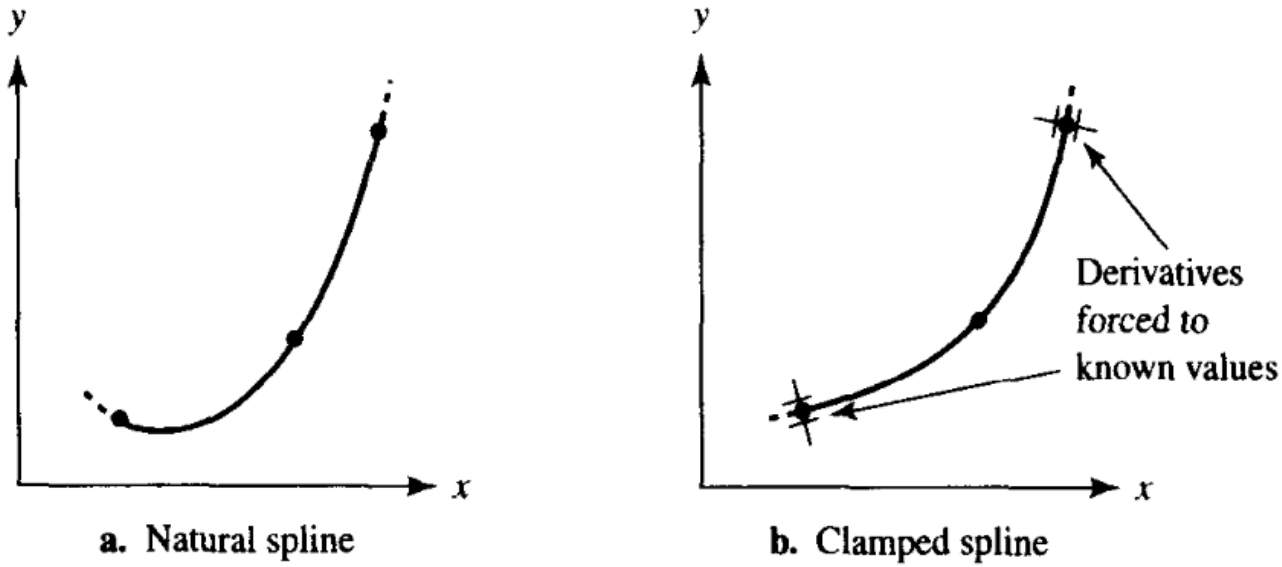
$$S_1(x_2) = y_2$$

$$S_2(x_2) = y_2$$

$$S_2(x_3) = y_3$$

约束条件

连接处导数约束: $S_1'(x_2) = S_2'(x_2),\ S_1''(x_2) = S_2''(x_2)$
端点约束 (自然样条): $S_1''(x_1) = 0,\ S_2''(x_3) = 0$
端点约束 (强制样条): $S_1'(x_1) = f'(x_1),\ S_2'(x_3) = f'(x_3)$

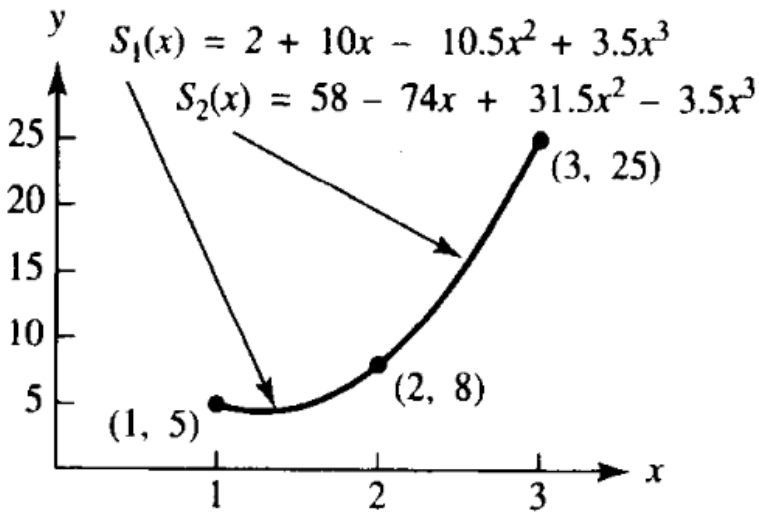


a. Natural spline

b. Clamped spline

拟合结果

Interval	Model
$1 \le x < 2$	$S_1(x) = 2 + 10x - 10.5x^2 + 3.5x^3$
$2 \le x \le 3$	$S_2(x) = 58 - 74x + 31.5x^2 - 3.5x^3$



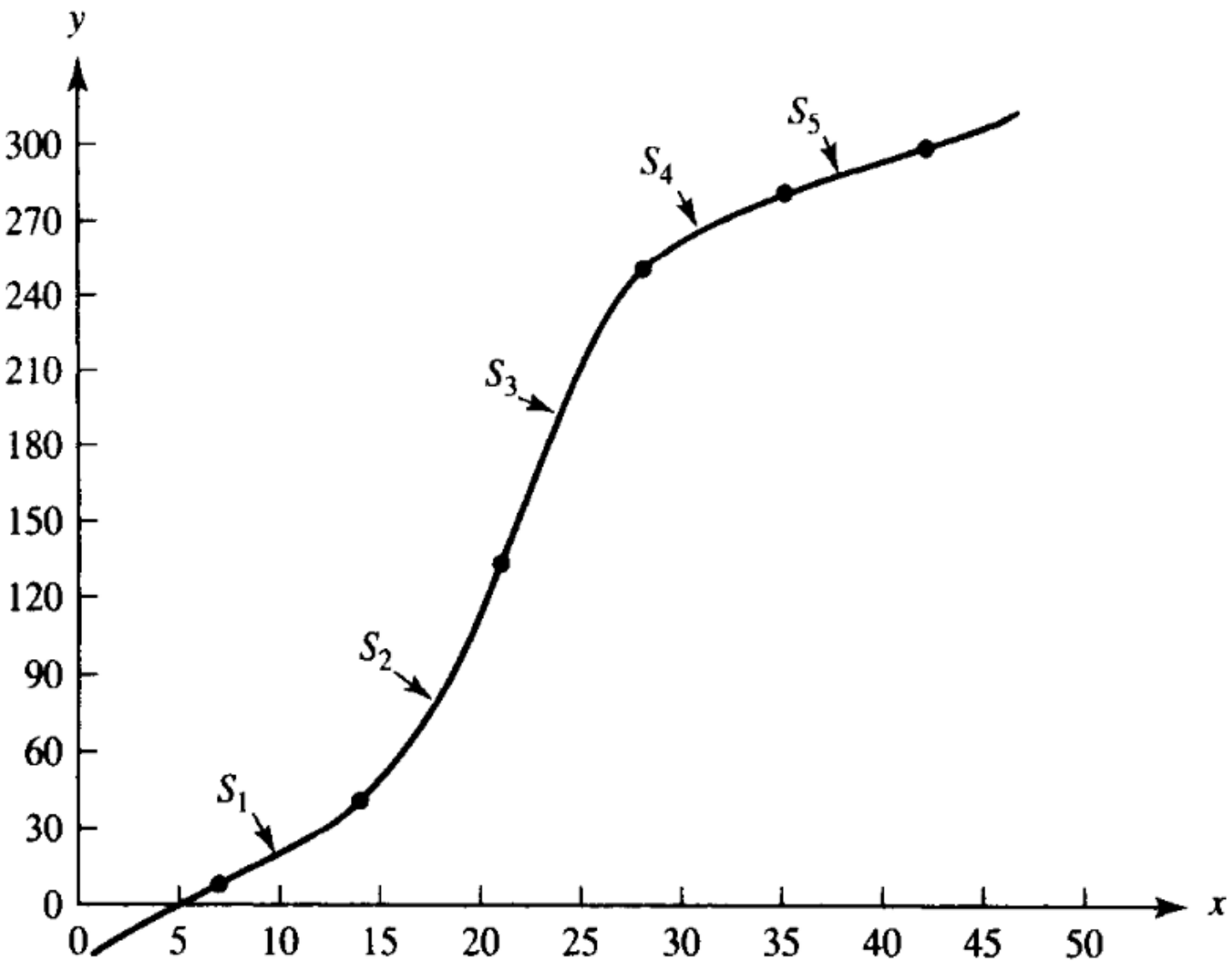
再论车辆的停止距离

Speed v (mph)	20	25	30	35	40	45	50	55	60	65	70	75	80
Distance d (ft)	42	56	73.5	91.5	116	142.5	173	209.5	248	292.5	343	401	464

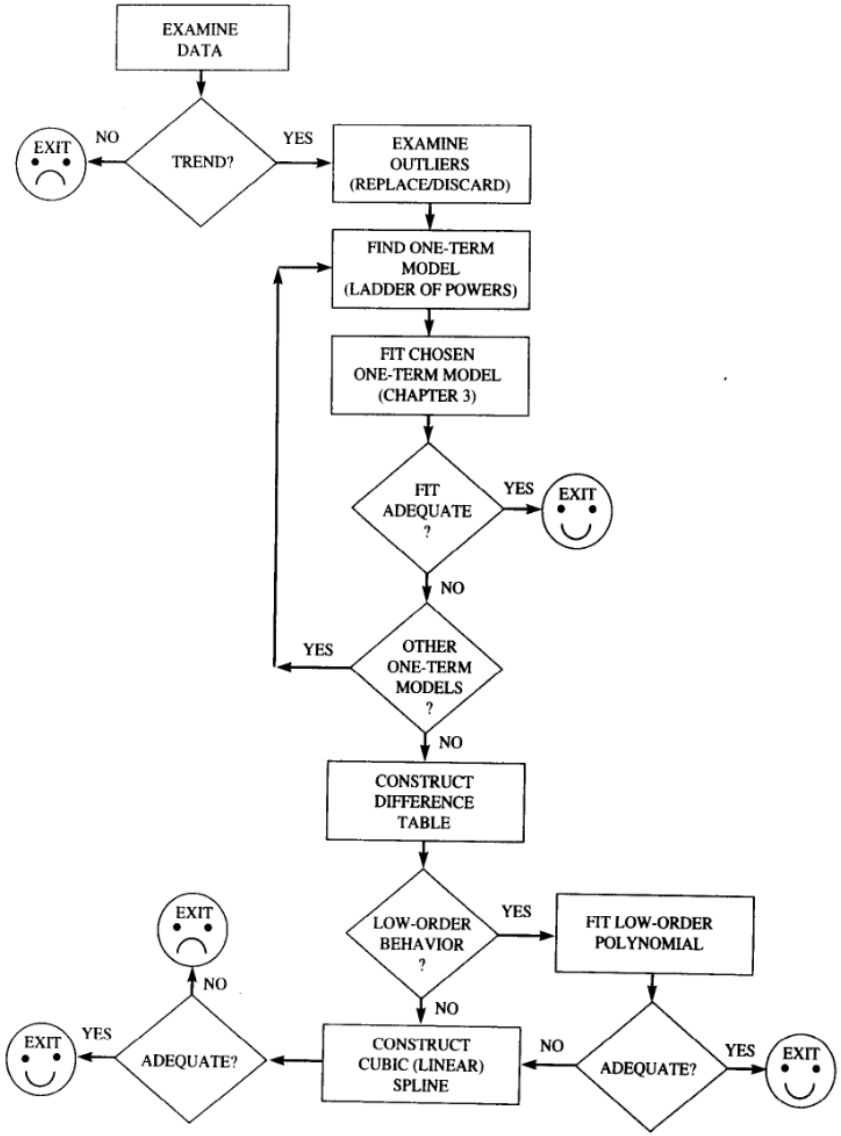
Interval	Model
$20 \le v < 25$	$S_1(v) = 42 + 2.596(v-20) + 0.008(v-20)^3$
$25 \le v < 30$	$S_2(v) = 56 + 3.208(v-25) + 0.122(v-25)^2 - 0.013(v-25)^3$
$30 \le v < 35$	$S_3(v) = 73.5 + 3.472(v-30) - 0.070(v-30)^2 + 0.019(v-30)^3$
$35 \le v < 40$	$S_4(v) = 91.5 + 4.204(v-35) + 0.216(v-35)^2 - 0.015(v-35)^3$
$40 \le v < 45$	$S_5(v) = 116 + 5.211(v-40) - 0.015(v-40)^2 + 0.006(v-40)^3$
$45 \le v < 50$	$S_6(v) = 142.5 + 5.550(v-45) + 0.082(v-45)^2 + 0.005(v-45)^3$
$50 \le v < 55$	$S_7(v) = 173 + 6.787(v-50) + 0.165(v-50)^2 - 0.012(v-50)^3$
$55 \le v < 60$	$S_8(v) = 209.5 + 7.503(v-55) - 0.022(v-55)^2 + 0.012(v-55)^3$
$60 \le v < 65$	$S_9(v) = 248 + 8.202(v-60) + 0.161(v-60)^2 - 0.004(v-60)^3$
$65 \le v < 70$	$S_{10}(v) = 292.5 + 9.489(v-65) + 0.096(v-65)^2 + 0.005(v-65)^3$
$70 \le v < 75$	$S_{11}(v) = 343 + 10.841(v-70) + 0.174(v-70)^2 - 0.005(v-70)^3$
$75 \le v < 80$	$S_{12}(v) = 401 + 12.245(v-75) + 0.106(v-75)^2 - 0.007(v-75)^3$

图: 三阶样条模型

拟合结果


y
300
270
240
210
180
150
120
90
60
30
0
0
5
10
15
20
25
30
35
40
45
50
x
S_1
S_2
S_3
S_4
S_5

构造经验模型


EXAMINE DATA
TREND?
NO
EXIT
YES
EXAMINE OUTLIERS (REPLACE/DISCARD)
FIND ONE-TERM MODEL (LADDER OF POWERS)
FIT CHOSEN ONE-TERM MODEL (CHAPTER 3)
FIT ADEQUATE ?
YES
EXIT
NO
OTHER ONE-TERM MODELS ?
YES
NO
CONSTRUCT DIFFERENCE TABLE
LOW-ORDER BEHAVIOR ?
YES
FIT LOW-ORDER POLYNOMIAL
NO
ADEQUATE?
YES
EXIT
NO
CONSTRUCT CUBIC (LINEAR) SPLINE
ADEQUATE?
YES
EXIT
NO
EXIT