Experimental Modeling

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Course outline

Curve fitting vs Interpolation

Curve fitting is to find a curve that could best indicate the trend of a given set of data. It allows some deviations between model and the collected data.

Interpolation is to connect discrete data points so that one can get reasonable estimates of data points between the given points. It connects all the data points using a (nonlinear) curve.

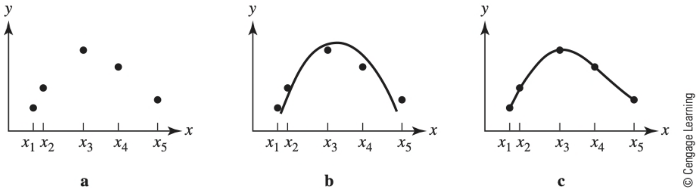


Figure 4.1

If the modeler expects a quadratic relationship, a parabola may be fit to the data, as in b. Otherwise, a smooth curve may be passed through the points, as in c.

Curve fitting vs Interpolation

Situation. If the modeler is unable to construct a tractable model form (curve fitting) that satisfactorily explains the behavior of the data, that is, the modeler does not know what kind of curve actually describes the behavior and if it is necessary to **predict** the behavior nevertheless, the modeler may conduct experiments (or otherwise gather data) to investigate the behavior of the dependent variable(s) for selected values of the independent variable(s) within some range. In essence, the modeler desires to construct an **empirical model** based on the collected data rather than select a model based on certain assumptions. In such cases the modeler is strongly influenced by the data that have been carefully collected and analyzed, so he or she seeks a curve (interpolation) that captures the trend of the data to predict in between the data points.

Harvesting in the Chesapeake Bay and Other One-Term Models

Let's consider a situation in which a modeler has collected some data but is unable to construct an explication model. In 1992, the Daily Press (a newspaper in Virginia) reported some observations (data) collected during the past 50 years on harvesting sea life in the Chesapeake Bay. We will examine several scenarios using observations from (a) harvesting bluefish and (b) harvesting blue crabs by the commercial industry of the Chesapeake Bay.

Table 4.1 Harvesting the bay, 1940–1990

Year	Bluefish (lb)	Blue crabs (lb)
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

Harvesting in the Chesapeake Bay and Other One-Term Models Cont.

Figure 4.2

Scatterplot of harvesting bluefish versus base year (5-year periods from 1940 to 1990)

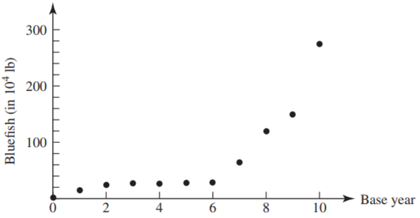
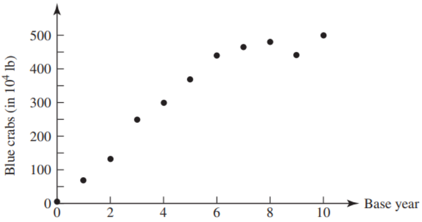


Figure 4.3

Scatterplot of harvesting blue crabs versus base year (5-year periods from 1940 to 1990)



Harvesting in the Chesapeake Bay and Other One-Term Models Cont.

- Figure 4.2 clearly shows a tendency to harvest more bluefish over time, indicating or suggesting the availability of bluefish. A more precise description is not so obvious.
- In Figure 4.3, the tendency is for the increase of harvesting of blue crabs. Again, a precise model is not so obvious.
- How we might begin to predict the availability of bluefish over time? Our strategy will be to transform the data of Table 4.1 in such a way that the resulting graph approximates a line, thus achieving a working model.
- But how do we determine the transformation?

Harvesting in the Chesapeake Bay and Other One-Term Models Cont.

Figure 4.4 shows a set of five data (x, y) with $y = x,\ \ x > 1.$

Suppose we change the y value of each point to $\sqrt{y},\ \log y, and\ \dfrac{1}{y}$

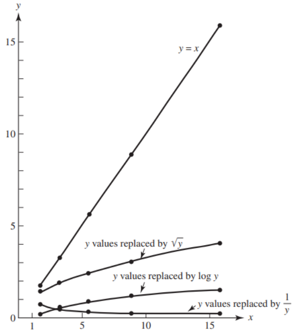


Figure 4.4: Relative effects of three transformation

Table 4.2 Ladder of Transformations

⋮
z^3
z^2
z (no change)
* $\left\{ \sqrt{z},\ \log z,\ \dfrac{-1}{\sqrt{z}},\ \dfrac{-1}{z} \right.$
$\dfrac{-1}{z^2}$
⋮

*The transformations most often used.

Harvesting in the Chesapeake Bay and Other One-Term Models Cont.

Example 1: Harvesting Bluefish

Recall from the scatterplot in Figure 4.2 that the trend of the data appears to be increasing and concave up. Using the ladder of powers to squeeze the right-hand tail downward, we can change y values by replacing y with $\log y$ or other transformations down the ladder. Another choice would be to replace x values with x^2 or x^3 values or other powers up the ladder.

- We fit with the least squares model of the form $\log y = mx + b$
- We obtain the model $\log y = 0.7231 + 0.1654x$ to data in **Table 4.3**
- The model can be written as $y = 5.2857(1.4635)^x$

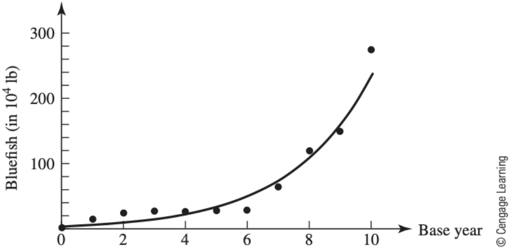
Table 4.3 Harvesting the bay: Bluefish, 1940–1990

Year	Base year x	Bluefish (lb) 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

Harvesting in the Chesapeake Bay and Other One-Term Models Cont.

Figure 4.5

Superimposed data and model $y = 5.2857(1.4635)^x$



Harvesting in the Chesapeake Bay and Other One-Term Models Cont.

Example 2: Harvesting Blue Crabs

Recall from our original scatterplot, Figure 4.3, that the trend of the data is increasing and concave down. With this information, we can utilize the ladder of transformations. We will use the data in Table 4.4, modified by making 1940 (year x = 0) the base year, with each base year representing a 5-year period.

- we can attempt to linearize these data by changing y values to y^2 or y^3 values or to others moving up the ladder.
- Replace the x values with $\sqrt{x}$
- Fit the model $y = k\sqrt{x}$ to data in **Table 4.4**
- Use least squares to find k, yielding

$$y = 158.344\sqrt{x}$$

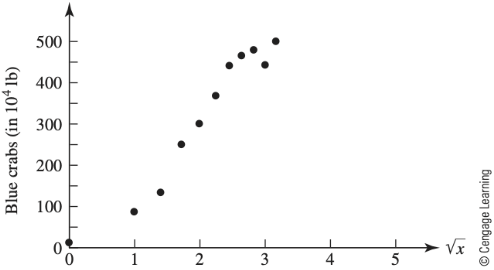
Table 4.4 Harvesting the bay: Blue crabs, 1940–1990

Year	Base year	Blue crabs (lb)
	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

Harvesting in the Chesapeake Bay and Other One-Term Models Cont.

Figure 4.6

Blue crabs (in 10^4 lb) versus $\sqrt{x}$



Harvesting in the Chesapeake Bay and Other One-Term Models Cont.

Figure 4.7

The line $y = 158.344\sqrt{x}$

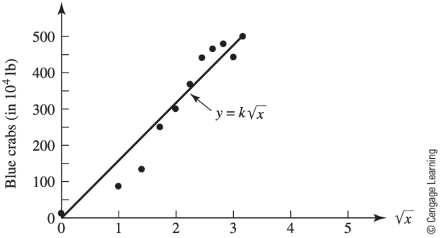
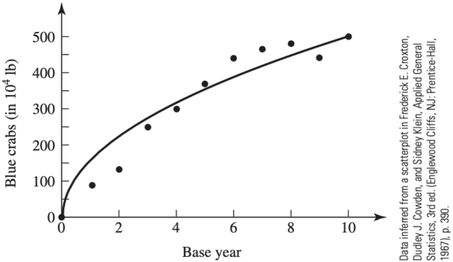


Figure 4.8

Superimposed data and model $y = 158.344\sqrt{x}$



High-Order Polynomial Models

- In some cases, models with a few terms may not be sufficient, hence models with more terms must be considered.
- Polynomial Model is one of the popular models as it is analytically easy to deal with.
- The polynomial models that pass through each point in a data set that includes only one observation for each value of the independent variable is called **polynomial interpolation**.

High-Order Polynomial Models

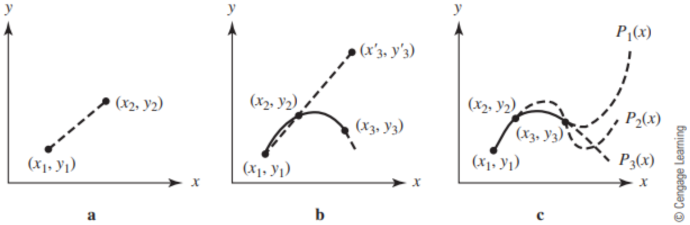


Figure 4.10

A unique polynomial of at most degree 2 can be passed through three data points (**a** and **b**), but an infinite number of polynomials of degree greater than 2 can be passed through three data points (**c**)

High-Order Polynomial Models Cont.

Consider the data

- In Figure 4.10 a, A unique line of $y = a_0 + a_1 x$ can be passed through (x_1, y_1) and (x_2, y_2). Determine the constant a_0 and a_1.
  By the conditions we obtain
  $$y_1 = a_0 + a_1 x_1$$
  and
  $$y_2 = a_0 + a_1 x_2$$
- In Figure 4.10 b, A unique polynomial function of (at most) degree 2, $y = a_0 + a_1 x + a_2 x^2$, can be passed through (x_1, y_1), (x_2, y_2) and (x_3, y_3). Determine the constant a_0, a_1 and a_2.
  By condition, we can find a_0, a_1 and a_2 by solving the following system of linear equations:
  $$\begin{aligned} y_1 &= a_0 + a_1 x_1 + a_2 x_1^2 \\ y_2 &= a_0 + a_1 x_2 + a_2 x_2^2 \\ y_3 &= a_0 + a_1 x_3 + a_2 x_3^2 \end{aligned}$$

High-Order Polynomial Models Cont.

Example. Elapsed Time of a Tape Recorder

Let's construct an empirical model to predict the amount of elapsed time of a tape recorder as a function of its counter reading. Let c_i represent the counter reading and t_i (sec) the corresponding amount of elapsed time. Consider the following data:

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

- One empirical model is a polynomial that pass through each of the data point. Since we have 8 data point, so a unique polynomial of at most 7 degree as following

$$P_7(c) = a_0 + a_1c + a_2c^2 + a_3c^3 + a_4c^4 + a_5c^5 + a_6c^6 + a_7c^7$$

- The eight data points require that the constants a_i satisfy the following system of linear algebraic equations:

High-Order Polynomial Models Cont.

$$205 = a_0 + 1a_1 + a_1^2 2 + 1^3 a_3 + 1^4 a_4 + 1^5 a_5 + 1^6 a_6 + 1^7 a_7$$
$$430 = a_0 + 2a_1 + 2^2 a_2 + 2^3 a_3 + 3^4 a_4 + 5^5 a_5 + 2^6 a_6 + 2^7 a_7$$
$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$
$$222 = a_0 + 8a_1 + 8^2 a_2 + 8^3 a_3 + 8^4 a_4 + 8^5 a_5 + 8^6 a_6 + 8^7 a_7$$

- We divide each counter reading of above system of linear algebraic equation by 100 to lessen the numerical difficulties. We get:

$$a_0 = -13.9999923 \qquad a_4 = -5.354166491$$
$$a_1 = 232.9119031 \qquad a_5 = 0.8013888621$$
$$a_2 = -29.08333188 \qquad a_6 = -0.0624999978$$
$$a_3 = 19.78472156 \qquad a_7 = 0.00198412222269$$

- Let's see how well the empirical model fits the data. Denoting the polynomial prediction by $P_7(c_i)$, we find

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

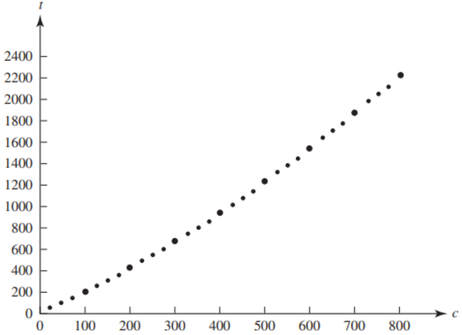
High-Order Polynomial Models Cont.

Can we really consider this model to be better than other model we could propose?

Let's see how well this new model $P_7(c_i)$ captures the trend of the data. The model is graphed in Figure 4.11.

Figure 4.11

An empirical model for predicting the elapsed time of a tape recorder



High-Order Polynomial Models Cont.

Theorem 1: Lagrangian Form of the Polynomial

If $x_0, x_1, \cdots, x_n$ are $(n+1)$ distinct points and $y_0, y_1, \cdots, y_n$ are corresponding observations at these points, then there exists a unique polynomial $P(x)$, of at most degree n, with the property that

$$y_k = P(x_k), \text{ for each } k = 0, 1, \cdots, n.$$

This polynomial is given by

$$P(x) = y_0 L_0(x) + \cdots + y_n L_n(x) \tag{4.3}$$

where

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

(4.3) passes through each of the data points, the resultant sum of absolute deviation is zero. Considering the various criteria of best fit presented in Chapter 3, we are tempted to use high-order polynomials to fit larger sets of data.

High-Order Polynomial Models Cont.

After all, the fit is precise. Let's examine both the advantages and the disadvantages of using high-order polynomials.
Suppose the following data have been collected:

x	x_1	x_2	x_3	x_4
y	y_1	y_2	y_3	y_4

By Theorem 1, we obtain cubic polynomial function:

$$\begin{aligned} P_3(x) = &\frac{(x-x_2)(x-x_3)(x-x_4)}{(x_1-x_2)(x_1-x_3)(x_1-x_4)}y_1 + \frac{(x-x_1)(x-x_3)(x-x_4)}{(x_2-x_1)(x_2-x_3)(x_2-x_4)}y_2 \\ &+ \frac{(x-x_1)(x-x_2)(x-x_4)}{(x_3-x_1)(x_3-x_2)(x_3-x_4)}y_3 + \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_4-x_1)(x_4-x_2)(x_4-x_3)}y_4 \end{aligned}$$

Convince yourself that the polynomial is indeed cubic and agrees with the value y_i when $x = x_i$. Notice that the x_i values must all be different to avoid division by zero. Observe the pattern for forming the numerator and the denominator for the coefficient of each y_i. This same pattern is followed when forming polynomials of any desired degree.

High-Order Polynomial Models Cont.

Advantages and Disadvantages of High-Order Polynomials

1. **Advantages**
   - Easy to estimate the coefficients of the polynomial
   - Calculus (computing derivative and integral) is easy with polynomial
2. **Disadvantages**
   - High-order polynomials may oscillate severely near the endpoints of the interval, a serious disadvantage to using them.
   - the polynomial can change quickly from increasing to decreasing, also making interpolation questionable.

See an example below.

High-Order Polynomial Models Cont.

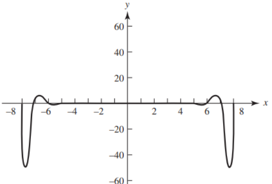
Consider some of the disadvantages of higher-order polynomials. For the 17 data points presented in Table 4.10, it is clear that the trend of the data is $y = 0$ for all x over the interval $-8 \leq x \leq 8$

Table 4.10

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

Suppose Equation (4.3) is used to determine a polynomial that passes through the points. Because there are 17 distinct data points, it is possible to pass a unique polynomial of degree at most 16 through the given points. The graph of a polynomial passing through the data points is depicted in Figure 4.12.

Figure 4.12
Fitting a higher-order polynomial through the data points in Table 4.10



Smoothing: Low-Order Polynomial Models

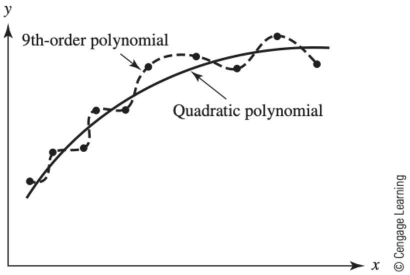
- We seek methods that retain many of the conveniences found in high-order polynomials without incorporating their disadvantages.
- One popular technique is to choose a low-order polynomial regardless of the number of data points.
- However, this choice normally results in a situation in which the number of data points exceeds the number of constants necessary to determine the polynomial.
- Low-order polynomials may not pass through all the data points.
- The process of finding low-order polynomial that best fits the data is call **polynomial smoothing**.
- This type of smoothing reduces both the tendency of the polynomial to oscillate and its sensitivity to small changes in the data.

Smoothing: Low-Order Polynomial Models

Figure 4.16 illustrates **quadratic smoothing** for 10 data points. This quadratic function smooths the data because it is not required to pass through all the data points.

Figure 4.16

The quadratic function smooths the data because it is not required to pass through all the data points.



Smoothing: Low-Order Polynomial Models

Example. Elapsed Time of a Tape Recorder Revisited

Find the quadratic smoothing polynomial: $P_2(c) = a + bc + dc^2$ for the following data

Table 4.13 Data collected for the tape recorder problem

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

Solution. To find the coefficients a, b, d, we use least squares method:

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

Smoothing: Low-Order Polynomial Models

Example. Elapsed Time of a Tape Recorder Revisited

The necessary conditions for a minimum to exist ($\partial S/\partial a = \partial S/\partial b = \partial S/\partial d = 0$) yield the following equations:

$$
\begin{aligned}
ma + \left(\sum c_i\right) b + \left(\sum c_i^2\right) d &= \sum t_i \\
\left(\sum c_i\right) a + \left(\sum c_i^2\right) b + \left(\sum c_i^3\right) d &= \sum c_i t_i \\
\left(\sum c_i^2\right) a + \left(\sum c_i^3\right) b + \left(\sum c_i^4\right) d &= \sum c_i^2 t_i
\end{aligned}
$$

For the data given in Table 4.13, the preceding system of equations becomes

$$
\begin{aligned}
8a + 3600b + 2{,}040{,}000d &= 9128 \\
3600a + 2{,}040{,}000b + 1{,}296{,}000{,}000d &= 5{,}318{,}900 \\
2{,}040{,}000a + 1{,}296{,}000{,}000b + 8.772 \times 10^{11} d &= 3{,}435{,}390{,}000
\end{aligned}
$$

Solution of the preceding system yields the values $a = 0.14286$, $b = 1.94226$, and $d = 0.00105$, giving the quadratic

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

Smoothing: Low-Order Polynomial Models

Example. Elapsed Time of a Tape Recorder Revisited

We can compute the deviation between the observations and the predictions made by the model $P_2(c)$:

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

Note that the deviations are very small compared to the order of magnitude of the times.

When we are considering the use of a low-order polynomial for smoothing, two issues come to mind:

1. Should a polynomial be used?
2. If so, what order of polynomial would be appropriate?

The derivative concept can help in answering these two questions.

Smoothing: Low-Order Polynomial Models

Divided Differences

Notice that a quadratic function is characterized by the properties that its second derivative is constant and its third derivative is zero. That is, given

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

we have

$$\begin{aligned} P'(x) &= b + 2cx \\ P''(x) &= 2c \\ P'''(x) &= 0 \end{aligned}$$

However, the only information available is a set of discrete data points. How can these points be used to estimate the various derivatives? Refer to Figure 4.17, and recall the definition of the derivative:

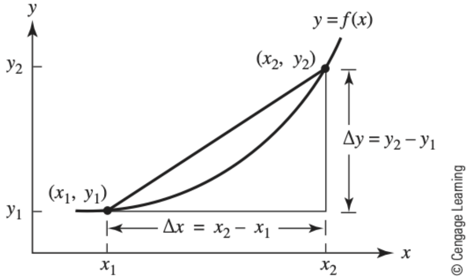
$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x}$$

Smoothing: Low-Order Polynomial Models

Divided Differences

Figure 4.17

The derivative of $y = f(x)$ at $x = x_1$ is the limit of the slope of the secant line.



If $\Delta x = x_2 - x_1$ is small, then

$$\frac{dy}{dx}(x_1) \approx \frac{\Delta y}{\Delta x} = \frac{y_2 - y_1}{x_2 - x_1}$$

Smoothing: Low-Order Polynomial Models

Divided Differences

If we have 3 data points, we can then estimate d^2y/dx^2 at $x = x_1$ by the second divided differences as illustrated in the following table:

Table 4.16 The first and second divided differences estimate the first and second derivatives, respectively

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

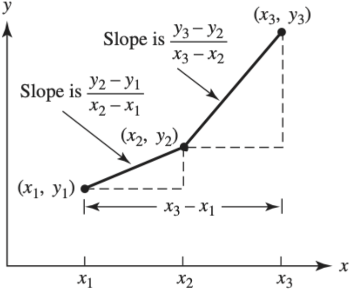
Smoothing: Low-Order Polynomial Models

Divided Differences

For graphic representation of the estimation of second derivative, see Figure 4.18 below.

Figure 4.18

The second divided difference may be interpreted as the difference between the adjacent slopes (first divided differences) divided by the length of the interval over which the change has taken place.



Smoothing: Low-Order Polynomial Models

Divided Differences: Example 1

Notation. Denote Δ^n, the nth divided difference that is used to estimate $d^n y/dx^n$. For the following data:

Table 4.14 A hypothetical set of collected data

x_i	0	2	4	6	8
y_i	0	4	16	36	64

then, we have the following estimate:

Table 4.17 A divided difference table for the data of Table 4.14

	Data		Divided differences		
	x_i	y_i	Δ	Δ^2	Δ^3
	0	0			
			$4/2 = 2$		
$\Delta x = 6$	2	4		$4/4 = 1$	
			$12/2 = 6$		$0/6 = 0$
	4	16		$4/4 = 1$	
			$20/2 = 10$		$0/6 = 0$
	6	36		$4/4 = 1$	
			$28/2 = 14$		
	8	64			

For this data, we will choose polynomial of degree 2 as smoothing model (as the 3rd derivative is 0).

Smoothing: Low-Order Polynomial Models

Divided Differences: Example 2. Elapsed Time of a Tape Recorder Revisited Again

Recall the data from Table 4.13. The divided differences are displayed in Table 4.18.

Table 4.18 A divided difference table for the tape recorder data

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				

For this data, choosing polynomial of degree 2 as smoothing model (as the 3rd derivative is 0) is appropriate.

Smoothing: Low-Order Polynomial Models

Divided Differences: Example 3. Vehicular Stopping Distance

Consider the following data:

Table 4.19 Data relating total stopping distance and speed

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

For this data, choosing polynomial of degree 2 as smoothing model (as the 3rd derivative is close to 0) is suggested. See Figure 4.20.

Smoothing: Low-Order Polynomial Models

Divided Differences: Example 3. Vehicular Stopping Distance

Table 4.20 A divided difference table for the data relating total vehicular stopping distance and speed

Data v_i	Data d_i	Divided differences 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				

Cubic Spline Models

Cubic Spline Interpolation

- A very much popular modern technique
- Preserve continuity
- Preserve smoothness up to second derivative (that is the model is of class C^2)
- Unlike polynomial smoothing, cubic spline can deal with oscillation problem.
- But, what is called **Spline**?

Cubic Spline Models

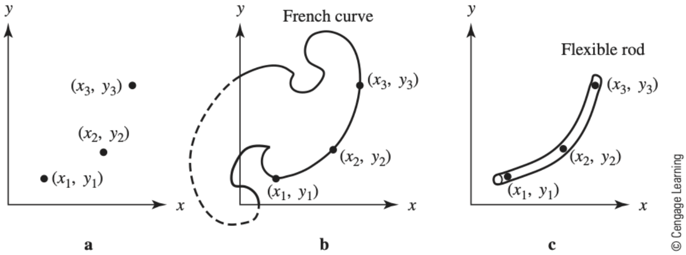


Figure 4.21

A draftsperson might attempt to draw a smooth curve through the data points using a French curve or a thin flexible rod called a *spline*.

Cubic Spline Models Cont.

Linear Interpolation

Linear interpolation take two (x_a, y_a), and (x_b, y_b) and the interpolation function at the point (x,y) is given by the following formula:

$$y = y_a + (y_b - y_a)\frac{x - x_a}{x_b - x_a}$$

Or similarly

$$y = a_1 + b_1 x$$

So if the above data is given in an ascending order, the linear splines are given by $(y_i = s(x_i))$

Use the Figure 4.22 and the data in Table 4.23 to generate a unique linear spline

Cubic Spline Models

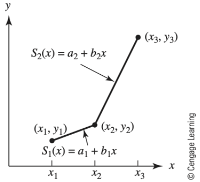
Linear Splines

- We start off by introducing **linear spline**.
- Suppose we have three points: $(x_1,\ y_1),\ (x_2,\ y_2),\ (x_3,\ y_3)$ given in the table below. We want to connect these points by piecewise linear functions, that is, from $x_1 \le x \le x_2$ by $S_1(x) = a_1 + b_1 x$ and from $x_2 \le x \le x_3$ by $S_2(x) = a_2 + b_2 x$.
- The overall graph is continuous.

Table 4.23
Linear interpolation

x_i	$y(x_i)$
1	5
2	8
3	25

Figure 4.22
A linear spline model is a continuous function consisting of line segments.



Cubic Spline Models

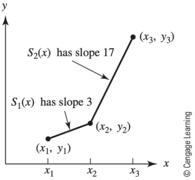
Linear Splines

By solving coordinates equations (there are four equations), we have:

Table 4.24 A linear spline model for the data of Table 4.23

Interval	Spline model
$1 \le x < 2$	$S_1(x) = 2 + 3x$
$2 \le x \le 3$	$S_2(x) = -26 + 17x$

Figure 4.23
The linear spline does not appear smooth because the first derivative is not continuous.



Cubic Spline Models

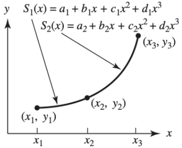
Cubic Splines

- Similar procedure to **linear spline**
- Suppose we have three points: $(x_1,\ y_1)$, $(x_2,\ y_2)$, $(x_3,\ y_3)$ given in the table below. We want to connect these points by piecewise linear functions, that is, from $x_1 \leq x \leq x_2$ by $S_1(x) = a_1 + b_1x + c_1x^2 + d_1x^3$ and from $x_2 \leq x \leq x_3$ by $S_2(x) = a_2 + b_2x + c_2x^2 + d_2x^3$.
- The overall graph is continuous, smooth and of class C^2.

Table 4.23 Linear interpolation

x_i	$y(x_i)$
1	5
2	8
3	25

Figure 4.24 A cubic spline model is a continuous function with continuous first and second derivatives consisting of cubic polynomial segments.



Cubic Spline Models Cont.

Cubic Splines Definition

Given $(x_1,\ y_1), (x_2,\ y_2), \cdots, (x_n,\ y_n)$ where $x_i, i = 1, 2, ..., n$ are distinct and in increasing order. A cubic spline $S(x)$ through the data points $(x_1, y_1), \cdots, (x_n, y_n)$ is a set of cubic polynomials:

$$S_1(x) = a_1 + b_1 x + c_1 x^2 + d_1 x^3 \text{ for } x \in [x_1, x_2]$$

$$S_2(x) = a_2 + b_2 x + c_2 x^2 + d_2 x^3 \text{ for } x \in [x_2, x_3]$$

$$\vdots$$

$$S_{n-1}(x) = a_{n-1} + b_{n-1} x + c_{n-1} x^2 + d_{n-1} x^3 \text{ for } x \in [x_{n-1}, x_n]$$

With the following conditions (known as properties):

a. $S_i(x_i) = y_i$ and $S_i(x_{i+1}) = y_{i+1}$ for $i = 1, 2, \ldots, n-1$.
   This property guarantees that the spline $S(x)$ interpolates the data points.

b. $S'_{i-1}(x_i) = S'_i(x_i)$ for $i = 2, 3, \ldots, n-1$.
   $S(x)$ is continuous on the interval $[x_1, x_n]$; this property forces the slopes of neighboring parts to agree when they meet.

Cubic Spline Models Cont.

Cubic Splines Definition Cont.

- $S''_{i-1}(x_i) = S''_i(x_i)$ for $i = 2, 3, \ldots, n-1$.
  $S''(x)$ is continuous on $[x_1, x_n]$, which also forces the neighboring spline to have the same curvature, to guarantee the smoothness.

Construction of cubic spline

How to determine the unknown coefficients a_i, b_i, c_i, and $d_i,\ i = 1, 2, \ldots, n-1$ of the cubic spline $S(x)$ so that we can construct it?
Given $S(x)$ is a cubic spline that has all the properties as in the definition.

$$S_i(x) = a_i + b_i x + c_i x^2 + d_i x^3, \text{on } [x_i, x_{i+1}],\ i = 1, 2, \ldots, n-1. \quad (1)$$

Cubic Spline Models Cont.

Construction of cubic spline Cont.

The first and second derivative:

$$S_i'(x) = b_i + 2c_i x + 3d_i x^2,\ i = 1, 2, \ldots, n-1. \tag{2}$$

$$S_i''(x) = 2c_i + 6d_i x,\ i = 1, 2, \ldots, n-1. \tag{3}$$

From the first property of cubic spline, $S(x)$ will interpolate all the data points, and we can have

$$S_i(x_i) = y_i$$

Since the curve $S(x)$ must be continuous across its entire interval, it can be concluded that each sub-function must join at the data points

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

Therefore,

$$y_i = S_{i-1}(x_i)$$

$$S_{i-1}(x_i) = a_{i-1} + b_{i-1}x + c_{i-1}x^2 + d_{i-1}x^3 \tag{4}$$

$$y_i = a_{i-1} + b_{i-1}x_i + c_{i-1}x_i^2 + d_{i-1}x_i^3, \quad i = 2, 3, \ldots, n. \tag{5}$$

Cubic Spline Models Cont.

Construction of cubic spline Cont.

Also, with properties 2 of cubic spline, the derivatives must be equal at the data points, that is

$$S'_{i-1}(x_i) = S'_i(x_i) \tag{6}$$

By eq(2), we obtain,

$$\begin{aligned} b_{i-1} + 2c_{i-1}x_i + 3d_{i-1}x_i^2 &= b_i + 2c_i x_i + 3d_i x_i^2 \\ b_i - b_{i-1} + 2(c_i - c_{i-1})x_i + 3(d_i - d_{i-1})x_i^2 &= 0 \end{aligned} \tag{7}$$

Since $S''_i(x)$ should be continuous across the interval, therefore

$$S''_{i-1}(x_i) = S''_i(x_i),$$

we obtain

$$\begin{aligned} 2c_{i-1} + 6d_{i-1}x_i &= 2c_i + 6d_i x_i \\ 2(c_i - c_{i-1}) + 6(d_i - d_{i-1})x_i &= 0 \end{aligned} \tag{8}$$

Cubic Spline Models Cont.

Construction of cubic spline Cont.

To determine unique constants, we still require two additional independent equations. We want second derivative at each endpoint (x_1 and x_n) to be 0, then

$$S_1''(x_1) = 2c_1 + 6d_1x_1 = 0 \tag{9}$$

$$S_{n-1}''(x_n) = 2c_{n-1} + 6d_{n-1}x_n = 0 \tag{10}$$

A cubic spline formed in this manner is called a **natural spline**.
Alternatively, if the values of the first derivative at the exterior endpoints are known, the first derivatives of the exterior splines can be required to match the known values. Suppose the derivatives at the exterior endpoints (x_1 and x_n) are known and are given by $f'(x_1)$and $f'(x_n)$. we obtain

$$S_1'(x_1) = b_1 + 2c_1x_1 + 3d_1x_1^2 = f'(x_1)$$

$$S_{n-1}'(x_n) = b_{n-1} + 2c_{n-1}x_n + 3d_{n-1}x_n^2 = f'(x_n)$$

A cubic spline formed in this manner is called **a clamped spline.**

Cubic Spline Models Cont.

Example of cubic spline

Generate the unique cube spline $S(x)$ to pass through the points $(1, 5), (2, 8)$ and $(3, 28)$.

- The cubic spline $S(x)$ such as:

$$S_1(x) = a_1 + b_1 x + c_1 x^2 + d_1 x^3$$
$$S_2(x) = a_2 + b_1 + x + c_2 x^2 + d_2 x^3$$

- The Spline $S_1(x)$ to pass through the two $(1, 5)$ and $(2, 8)$ of its interval requires that $S_1(1) = 5$ and $S_1(2) = 8$

$$a_1 + 1b_1 + 1c_1 + 1d_1 = 5 \tag{11}$$
$$a_1 + 2b_1 + 2^2 c_1 + 2^3 d_1 = 8 \tag{12}$$

- Similarly, $S_2(x)$ must pass through its endpoint of the second interval so that $S_2(2) = 8$ and $S_2(3) = 25$ or

$$a_2 + 2b_2 + 2^2 c + 2 + 2^3 d_2 = 8 \tag{13}$$
$$a_2 + 3b_2 + 3^2 c_2 + 3^3 d_2 = 25 \tag{14}$$

Cubic Spline Models Cont.

- The first derivative of $S_1(x)$ and $S_2(x)$ are forced to math at the interior data point $x_2 = 2 : S_1'(2) = S_2'(2)$ or

$$b_1 + 2c_1(2) + 3d_1(2)^2 = b_2 + 2c_2(2) + 3d_2(2)^2 \tag{14}$$

- Forcing the second derivative of $S_1(x)$ and $S_2(x)$ to match at $x_2 = 2$ requires $S_1''(2) = S_2''(2)$ or

$$2c_1 + 6d_1(2) = 2c_2 + 6d_2(2) \tag{15}$$

- Finally, a natural spline is built by requiring that the second derivatives at the endpoints be zero: $S_1''(1) = S_2''(3) = 0$ or

$$2c_1 + 6d_1(1) = 0 \tag{16}$$
$$2c_2 + 6d_2(3) = 0 \tag{17}$$

Cubic Spline Models

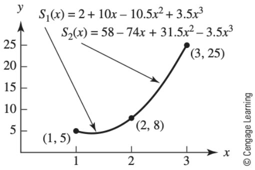
Cubic Splines

By solving coordinates equations and continuities equations of the first and second derivatives (there are in total eight equations), we have:

Table 4.25 A natural cubic spline model for the data of Table 4.23

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

Figure 4.26
The natural cubic spline model for the data in Table 4.23 is a smooth curve that is easily integrated and differentiated.



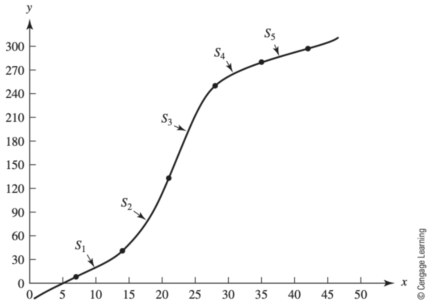
Cubic Spline Models

Example: Fitting with Cubic Splines

Fit the following data using cubic spline.

x	7	14	21	28	35	42
y	8	41	133	250	280	297

Figure 4.28
The smooth composite cubic spline from the cubic polynomials in Figure 4.27



Cubic Spline Models

Example: Model for Vehicular Stopping Distance. Fitting with Cubic Splines

Fit the following data using cubic spline.

Table 4.26 Data relating total stopping distance and speed

Speed, v (mph)	20	25	30	35	40	45	50
Distance, d (ft)	42	56	73.5	91.5	116	142.5	173

Speed, v (mph)	55	60	65	70	75	80
Distance, d (ft)	209.5	248	292.5	343	401	464

Cubic Spline Models

Example: Model for Vehicular Stopping Distance. Fitting with Cubic Splines

Solution.

Table 4.27 A cubic spline model for vehicular stopping distance

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

Cubic Spline Models

Example: Model for Vehicular Stopping Distance. Fitting with Cubic Splines

Graph.

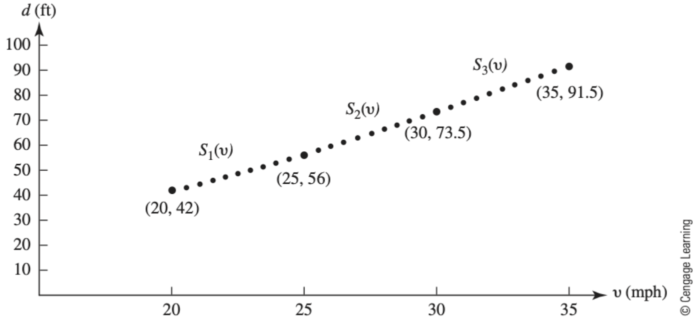


Figure 4.29

A plot of the cubic spline model for vehicular stopping distance for $20 \leq v \leq 35$

Cubic Spline Models

A flowchart for empirical model building

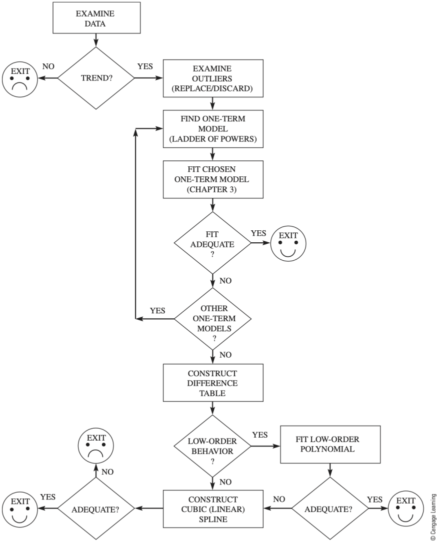


Figure 4.30
A flowchart for empirical model building