Experimental Modeling

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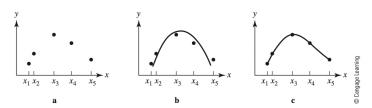
Course outline

- Introduction
- 2 Harvesting in the Chesapeake Bay and Other One-Term Models
- 3 High-Order Polynomial Models
- 4 Smoothing: Low-Order Polynomial Models
- **5** Cubic Spline Models

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.

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

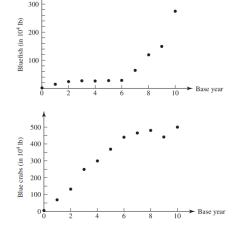
Year	Bluefish (lb)	Blue crabs (lb)			
1940	15,000	100,000			
1945	150,000	850,000			
1950	250,000	1,330,000			
1955	275,000	2,500,000			
1960	270,000	3,000,000			
1965	280,000	3,700,000			
1970	290,000	4,400,000			
1975	650,000	4,660,000			
1980	1,200,000	4,800,000			
1985	1,500,000	4,420,000			
1990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

■ 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)



- 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?

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 $\sqrt{y},\ \log y, and\ \frac{1}{y}$

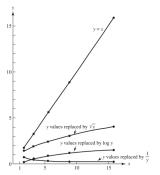


Figure 4.4: Relative effects of three transformation



*The transformations most often used

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.

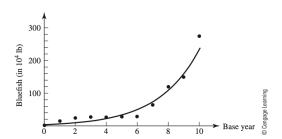
- We fit with the least squares model of the form $\log y = mx + b$
- We obtain the model $\log y = 0.7231 + 0.1654x$ to data in **Table 4.3**
- The model can be written as $y = 5.2857(1.4635)^x$

Table 4.3 Harvesting the bay: Bluefish, 1940-1990

Year	Base year	Bluefish (lb				
	x	у				
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				

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■ Figure 4.5 Superimposed data and model $y = 5.2857(1.4635)^x$



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 $\times = 0$) the base year, with each base year representing a 5-year period.

1990

- 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	у							
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							

■ Figure 4.6 Blue crabs (in 10^4 lb) versus \sqrt{x}

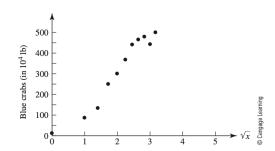
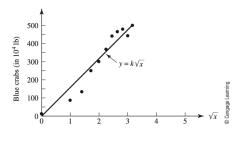


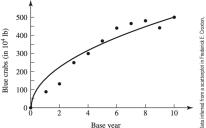
Figure 4.7

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

■ Figure 4.8

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

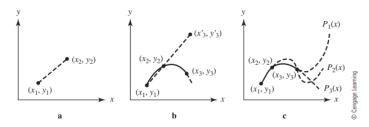




ta inferred from a scatterplot in Frederick E. Crox dley J. Cowden, and Sidney Klein, Applied Gener atistics, 3rd ed. (Englewood Cliffs, NJ: Prentice-H 67), p. 390.



- 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.



■ 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)

Consider the data

• In Figure 4.10 a, A unique line of $y=a_0+a_1x$ 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, $y=a_0+a_1x+a_2x^2$, 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:

$$y_1 = a_0 + a_1 x_1 + a_2 x_1^2$$
$$y_2 = a_0 + a_1 x_2 + a_2 x_2^2$$
$$y_3 = a_0 + a_1 x_3 + a_2 x_3^2$$

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

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

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

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

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

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

- 6					500			
t_i (sec)	205	430	677	945	1233	1542	1872	2224
$P_{\tau}(c_i)$	205	430	677	045	1233	1542	1872	2224

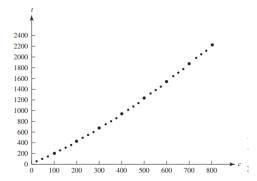


Can we really consider this model to be better than other model we could propose?

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



Theorem 1: Lagrangian Form of the Polynomial

If x_0, x_1, \dots, x_n are (n+1) distinct points and y_0, y_1, \dots, 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

$$y_k = P(x_k)$$
, for each $k = 0, 1, \dots, n$.

This polynomial is given by

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

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:

By Theorem 1, we obtain cubic polynomial function:

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

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.

Advantages and Disadvantages of High-Order Polynomials

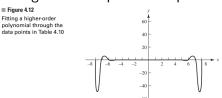
- Advantages
 - Easy to estimate the coefficients of the polynomial
 - Calculus (computing derivative and integral) is easy with polynomial
- ② Disadvantages
 - High-order polynomials may oscillate severely near the endpoints of the interval, a serious disadvantage to using them.
 - the polynomial can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

See an example below.

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 $-8 \le x \le 8$

Table	e 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.



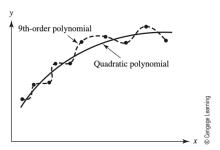


- We seek methods that retain many of the conveniences found in high-order polynomials without incorporating their disadvantages.
- One popular technique is to choose a low-order polynomial regardless of the number of data points.
- However, this choice normally results in a situation in which the number 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.

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.



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

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

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

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:

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

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

$$8a + 3600b + 2,040,000d = 9128$$
$$3600a + 2,040,000b + 1,296,000,000d = 5,318,900$$
$$2,040,000a + 1,296,000,000b + 8,772 \times 10^{11}d = 3,435,390,000$$

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

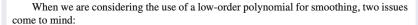
$$P_2(c) = 0.14286 + 1.94226c + 0.00105c^2$$

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
$\overline{t_i - P_2(c_i)}$	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.



- 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.

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

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

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

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

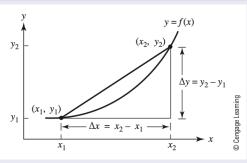
However, the only information available is a set of discrete data points. How can these points be used to estimate the various derivatives? Refer to Figure 4.17, and recall the definition of the derivative:

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

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

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

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

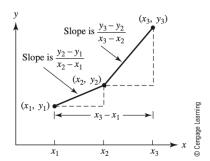
Data		First divided difference	Second divided difference				
x_1	у1	$\frac{y_2 - y_1}{x_2 - x_1}$					
<i>x</i> ₂	<i>y</i> ₂	72 71	$\frac{\frac{y_3 - y_2}{x_3 - x_2} - \frac{y_2 - y_1}{x_2 - x_1}}{x_3 - x_1}$				
<i>x</i> ₃	у3	$\frac{y_3 - y_2}{x_3 - x_2}$					

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.



Divided Differences: Example 1

Notation. Denote \triangle^n , the *n*th 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
yi	0	4	16	36	64

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then, we have the following estimate:

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

	Data	Di	vided difference	
x_i	y_i	Δ	Δ^2	Δ^3
$\Delta x = 6 \begin{cases} 2\\4\\6\\8 \end{cases}$ © Cengage Learning	0 4 16 36 64	4/2 = 2 $12/2 = 6$ $20/2 = 10$ $28/2 = 14$	4/4 = 1 4/4 = 1 4/4 = 1	0/6 = 0 0/6 = 0

For this data, we will choose

polynomial of degree 2 as smoothing model (as the 3rd derivative is 0).

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

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

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

Divided Differences: Example 3. Vehicular Stopping Distance

Consider the following data:

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
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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.

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		Divided differences			
v_i	d_i	Δ	Δ^2	Δ^3	Λ^4
20 25 30 35 40 45 50 55 60 65 70 75 80	42 56 73.5 91.5 116 142.5 173 209.5 248 292.5 343 401 464	2.2800 3.5000 3.6000 4.9000 5.3000 6.1000 7.3000 7.7000 8.9000 10.1000 11.6000 12.6000	0.0700 0.0100 0.1300 0.0400 0.0800 0.1200 0.1200 0.1200 0.1500 0.1000	-0.0040 0.0080 -0.0060 0.0027 0.0027 -0.0053 0.0053 0.0000 0.0020 -0.0033	0.0006 -0.0007 0.0002 -0.0002 -0.0003 -0.0003

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**?