Numerical Methods
Curve Fitting

by

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Description

AIMS

This chapter is an introduction to the numerical methods. It is aimed to:

1. introduce the curve fitting problem.
2. show how to approximate the value of certain data.
3. define the concept of interpolation and inverse interpolation

EXPECTED OUTCOMES

1. Students should be able to explain the Newton’s divided-difference table.
2. Students should be able to differentiate between interpolation and inverse interpolation.
3. Students should be able to identify linear and quadratic splines.
4. Students should be able to solve curve fitting problem using Newton interpolation method, Lagrange interpolation method, linear spline and quadratic spline.

REFERENCES

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Content

INTRODUCTION

INTERPOLATION

1

In science and engineering, one often has few known data points obtained through experiments and sampling.

2

Through the limited data points, one can estimate the result for certain value of independent variable by using interpolation method.

3

Interpolation is a method of constructing new data points within the range of discrete data set of known data points. It means estimating the value of $f(x)$ for a certain value of x, provided that x must lies within the range of the data set and the interval or step size of x points is not necessary to be equidistant.

INTRODUCTION (Cont.)

Given the data points that generated through the function $f(x) = \cos(2x + 1)$

Table 1: Data Generated from $f(x) = \cos(2x + 1)$

x	$f(x)$	x	$f(x)$
0	0.5403	2.0	0.2837
0.5	-0.4161	2.5	0.9602
1.0	-0.9900	3.0	0.7539
1.5	-0.6536		

INTRODUCTION (Cont.)

The data points given in **Table 1** can be plotted by using linear or curvilinear interpolation as illustrated in the **Figure 1**.

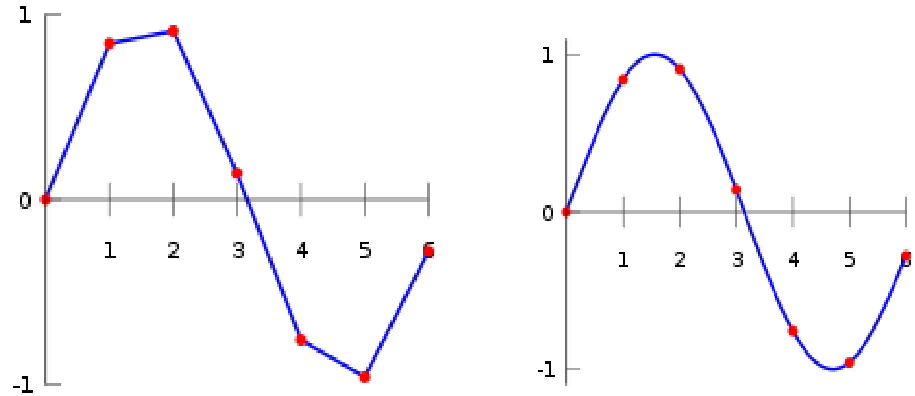

Figure 1: Linear and curvilinear interpolation of the data points.

In order to estimate the value of $f(2.4)$, a polynomial function for the respective data by using interpolation method.

INTRODUCTION (Cont.)

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INTERPOLATION METHODS

1

Polynomial interpolation which is divided into three; **Newton interpolation, Lagrange interpolation** and **Inverse interpolation.**

2

Spline and piecewise interpolation which is divided into two; **Linear** and **Quadratic splines**.

POLYNOMIAL INTERPOLATION

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Polynomial Interpolation

1. Polynomial Interpolation is the most common method used in practice.

2. There is only one polynomial of order n that passes through all the $n+1$ observations.

3. It refers to a method of determining the unique n^{th} order polynomial that is $n+1$ data points.

4. Two types of polynomial interpolation: Newton Interpolation and Lagrange Interpolation.

NEWTON INTERPOLATION METHOD

Newton Interpolation Method: General Form

The general formula for an n^{th} order polynomial is

$$f(x) = a_0 + a_1 x + a_2 x^2 + ... + a_n x^n$$

For $n + 1$ data points, there is one and only one polynomial of order n that passes through all the points.
Polynomial interpolation consists of determining the unique n^{th}-order polynomial that fits $n + 1$ data points. Suppose that the function $f(x)$ is tabulated at the points $x_0, x_1, \ldots, x_n$ where the x point is not necessary to be equidistant. the Newton interpolating polynomial of degree n can be written as

$$f_n(x) = f(x_0) + (x - x_0) f[x_0, x_1] + (x - x_0)(x - x_1) f[x_0, x_1, x_2]$$
$$+ \cdots + (x - x_0)(x - x_1) \cdots (x - x_{n-1}) f[x_0, \cdots, x_{n-1}, x_n]$$

where $f(x) = f[x_0, x_1], f[x_0, x_1, x_2], ..., f[x_0, x_1, ..., x_n]$ are Newton's divided difference that can be calculated using Table 2.

NEWTON INTERPOLATION METHOD (Cont.)

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Table 2: The Newton's Divided-Difference

x_i	$f(x_i)$	First divided differences	Second divided differences	Third divided differences
x_0	$f(x_0)$			
x_1	$f(x_1)$	$f[x_1,x_0]=\frac{f(x_1)-f(x_0)}{x_1-x_0}$		
x_2	$f(x_2)$	$f[x_2,x_1]=\frac{f(x_2)-f(x_1)}{x_2-x_1}$	$f[x_2,x_1,x_0]=\frac{f[x_2,x_1]-f[x_1,x_0]}{x_2-x_0}$	
x_3	$f(x_3)$	$f[x_3,x_2]=\frac{f(x_3)-f(x_2)}{x_3-x_2}$	$f[x_3,x_2,x_1]=\frac{f[x_3,x_2]-f[x_2,x_1]}{x_3-x_1}$	$f[x_3,x_2,x_1,x_0]=\frac{f[x_3,x_2,x_1]-f[x_2,x_1,x_0]}{x_3-x_0}$
x_4	$f(x_4)$	$f[x_4,x_3]=\frac{f(x_4)-f(x_3)}{x_4-x_3}$	$f[x_4,x_3,x_2]=\frac{f[x_4,x_3]-f[x_3,x_2]}{x_4-x_2}$	$f[x_4,x_3,x_2,x_1]=\frac{f[x_4,x_3,x_2]-f[x_3,x_2,x_1]}{x_4-x_1}$
x_5	$f(x_5)$	$f[x_5,x_4]=\frac{f(x_5)-f(x_4)}{x_5-x_4}$	$f[x_5,x_4,x_3]=\frac{f[x_5,x_4]-f[x_4,x_3]}{x_5-x_3}$	$f[x_5,x_4,x_3,x_2]=\frac{f[x_5,x_4,x_3]-f[x_4,x_3,x_2]}{x_5-x_2}$

NEWTON INTERPOLATION METHOD (Cont.)

Example 1

Given the data below.

x	1	5	9	13
$f(x) = \ln x$	0	1.609438	2.197225	2.564950

Based on the given data, estimate $\ln(7)$ using third-order Newton interpolating polynomial. Then, calculate the true percent relative error, ε_t.

NEWTON INTERPOLATION METHOD (Cont.)

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Solution

Step 1 Form a divided-difference table.

x	$f(x)$	1st Divided Difference	2nd Divided Difference	3rd Divided Difference
1	0			
5	1.609438	$\frac{1.609438-0}{5-1}$ $=0.40236$		
9	2.197225	$\frac{2.197225-1.609438}{9-5}$ $=0.14695$	$\frac{0.14695-0.40236}{9-1}$ $=-0.03192$	
13	2.564950	$\frac{2.564950-2.197225}{13-9}$ $=0.09193$	$\frac{0.09193-0.14695}{13-5}$ $=-0.006878$	$\frac{-0.006878-(-0.03192)}{13-1}$ $=0.002087$

NEWTON INTERPOLATION METHOD (Cont.)

Solution (Cont.)

Step 2

Compute the approximate solution:

$$f_3(x) = f(x_0) + (x - x_0) f[x_1, x_0] + (x - x_0)(x - x_1) f[x_2, x_1, x_0] + (x - x_0)(x - x_1)(x - x_2) f[x_3, x_2, x_1, x_0]$$

$$f_3(x) = 0 + (7-1)(0.40236) + (7-1)(7-5)(-0.03192) + (7-1)(7-5)(7-9)(0.002087) \approx 1.981032$$

Step 3

Compute the exact solution: $\ln(7) = 1.945910$.

Step 4

$$\varepsilon_t = \left| \frac{1.945910 - 1.981032}{1.945910} \right| \times 100\% = 1.8049\%$$

LAGRANGE INTERPOLATION POLYNOMIAL

Lagrange Interpolation Method: General Form

Lagrange interpolating polynomial is a reformulation of the Newton polynomial which avoids the computation of divided differences.

The function $f(x)$ is approximated by using

$$f_{n-1}(x) = \sum_{i=0}^{n} L_i(x)\, f(x_i)$$

where

$$L_i(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

is the Lagrange coefficient with n^{th} order of interpolation.

LAGRANGE INTERPOLATION POLYNOMIAL (Cont.)

Example 3

Estimate $f(2)$ by using Lagrange interpolation polynomial for the following data.

x	1	4	5	6
$f(x)$	2.0248	8.1915	11.3181	16.8020

LAGRANGE INTERPOLATION POLYNOMIAL (Cont.)

Solution

In this example, we are given four data points. Therefore, $n = 3$, that is we need to derive a cubic polynomial using Lagrange interpolation method. The formula of third order Lagrange interpolation is:

$$
\begin{aligned}
f_3(x) &= L_0 f(x_0) + L_1 f(x_1) + L_2 f(x_2) + L_3 f(x_3) \\
&= \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} f(x_0) + \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)} f(x_1) \\
&\quad + \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} f(x_2) + \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)} f(x_3)
\end{aligned}
$$

LAGRANGE INTERPOLATION POLYNOMIAL (Cont.)

Solution

INVERSE INTERPOLATION

INVERSE INTERPOLATION

1

Method of finding the value of x for a certain value of $f(x)$ which is inside the range of data set. This case is called inverse interpolation.

2

Newton divided-difference method and Lagrange interpolation methods are used but in reversed way.

INVERSE INTERPOLATION (Cont.)

Inverse Newton Interpolation Polynomial

The general Inverse Newton interpolation polynomial can be represented as

$$P_n(f) = x_0 + (f - f_0)\,x[f_1, f_0] + (f - f_0)(f - f_1)\,x[f_2, f_1, f_0] + \dots + (f - f_0)(f - f_1)\dots(f - f_{n-1})\,x[f_n, f_{n-1}, \dots, f_0]$$

where

$$x[f_n, f_{n-1}, \dots, f_0] = \frac{x[f_n, f_{n-1}, \dots, f_1] - x[f_{n-1}, f_{n-1}, \dots, f_0]}{f_n - f_0}$$

INVERSE INTERPOLATION (Cont.)

Inverse Lagrange Interpolation Polynomial

The general Inverse Lagrange interpolation polynomial can be represented as

$$P_n(f) = \sum_{i=0}^{n} L_i f(x_i)$$

where

$$L_i f(x_i) = \prod_{j=0,\, j\neq i}^{n} \frac{f - f_j}{f_i - f_j}$$

INVERSE INTERPOLATION (Cont.)

Example 4

The following table is generated through the function $f(x) = \frac{5}{x}$.

x	1	4	5	6
$f(x)$	2.0248	8.1915	11.3181	16.8020

Employ inverse interpolation to determine the value of x that correspond to $f(x) = 1.5$ for the above data by using

i) Newton interpolation method

ii) Lagrange interpolation method

Then, compute the true percent relative error for both methods. Use five decimal places in all calculations.

INVERSE INTERPOLATION (Cont.)

Solution

i) Inverse Newton interpolation method.

$$P_3(f) = x_0 + (f - f_0)x[f_1, f_0] + (f - f_0)(f - f_1)x[f_2, f_1, f_0]$$
$$+ (f - f_0)(f - f_1)(f - f_2)x[f_3, f_2, f_1, f_0]$$

$$P_3(f) = 3.2 + (1.5 - 1.5625)(-2.17628) + (1.5 - 1.5625)(1.5 - 1.4706)(1.5651)$$
$$+ (1.5 - 1.5625)(1.5 - 1.4706)(1.5 - 1.3889)(-1.19719)$$
$$= 3.33339$$

INVERSE INTERPOLATION (Cont.)

Solution

ii) Inverse Lagrange interpolation method

$$
\begin{aligned}
P_3(1.5) &= \frac{(1.5-1.4706)(1.5-1.3889)(1.5-1.3158)}{(1.5625-1.4706)(1.5625-1.3889)(1.5625-1.3158)}(3.2) \\
&+ \frac{(1.5-1.5625)(1.5-1.3889)(1.5-1.3158)}{(1.4706-1.5625)(1.4706-1.3889)(1.4706-1.3158)}(3.4) \\
&+ \frac{(1.5-1.5625)(1.5-1.4706)(1.5-1.3158)}{(1.3889-1.5625)(1.3889-1.4706)(1.3889-1.3158)}(3.6) \\
&+ \frac{(1.5-1.5625)(1.5-1.4706)(1.5-1.3889)}{(1.3158-1.5625)(1.3158-1.4706)(1.3158-1.3889)}(3.8) \\
&= 0.15287(3.2)+1.10046(3.4)-0.32646(3.6)+0.07313(3.8) \\
&= 3.33339
\end{aligned}
$$

SPLINE AND PIECEWISE INTERPOLATION

Introduction

- A high order polynomial interpolation might not be the best choice to interpolate between a large numbers of data points because of erroneous results due to round-o error and overshoot.
- A higher-order polynomial tends to swing through wild oscillations in the vicinity of abrupt change (see Figure 2).

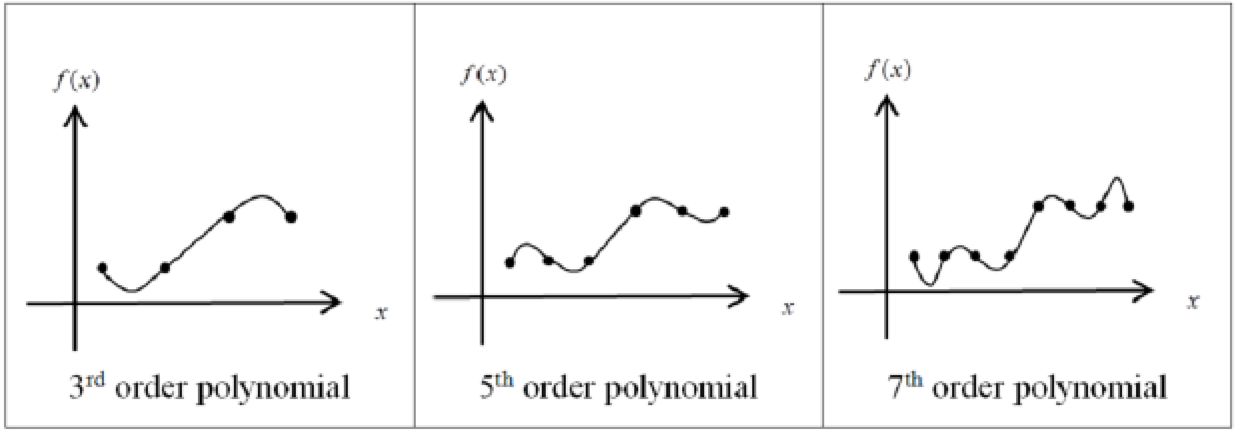


Figure 2: Abrupt changes of the function as the order of polynomial gets higher.

SPLINES AND PIECEWISE INTERPOLATION (Cont.)

Introduction (Cont.)

- An alternative approach which apply lower order polynomials to subsets of data points is required to interpolate the value of $f\ (x)$ for large number of data.
- This approach is called spline interpolation method. Spline polynomial often performs better than higher degree polynomials.
- As in Figure 3, spline performs better because it kept the oscillations to a minimum by using small subsets of points for each interval rather than every point.

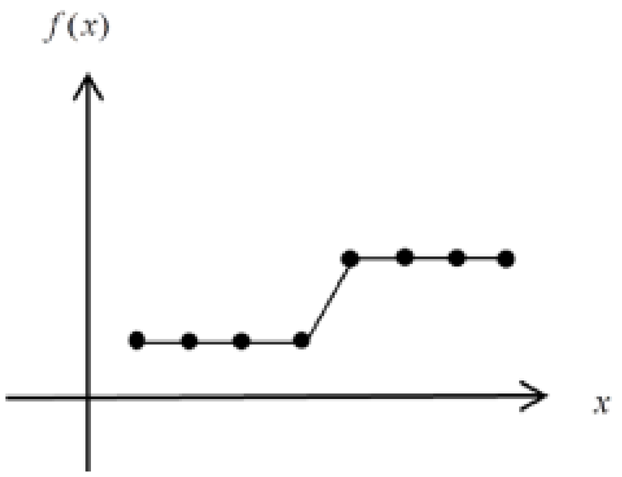
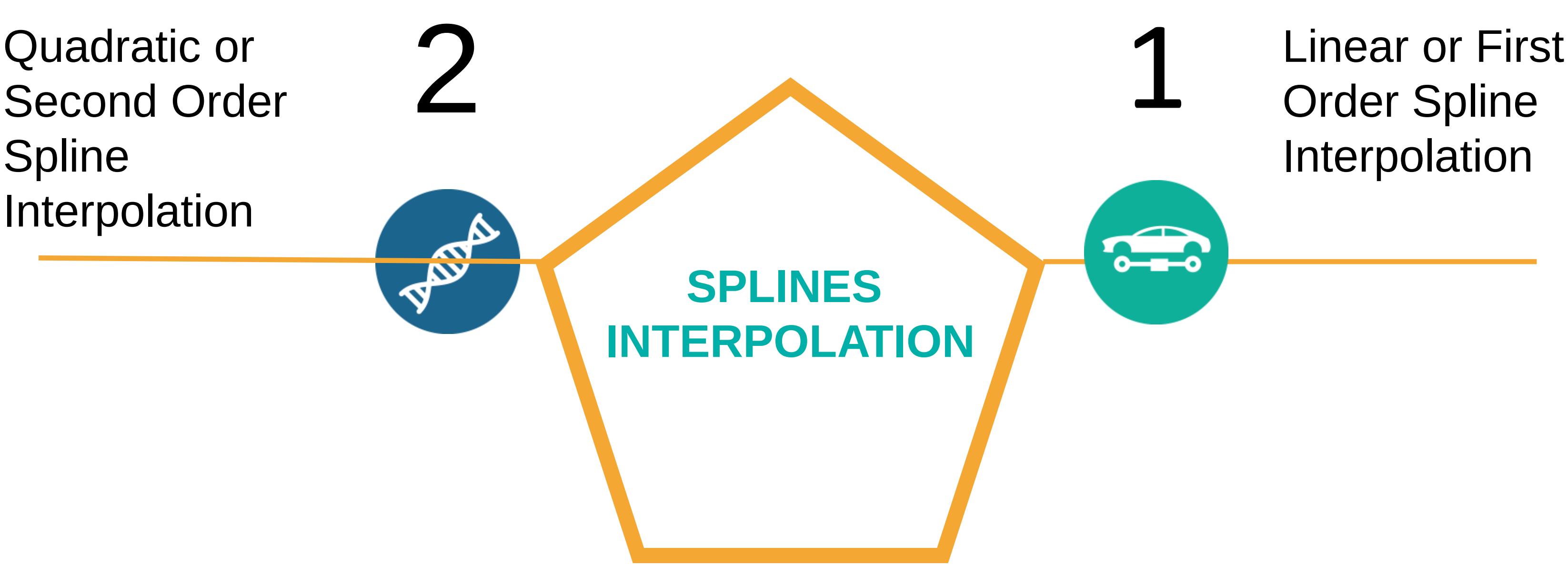


Figure 3: First-order polynomials generated through spline interpolation for seven data points

SPLINES AND PIECEWISE INTERPOLATION (Cont.)

Introduction (Cont.)



LINEAR SPLINE

Introduction

In the first-order spline, basically we are finding the straight line equations connecting each pair of interval (x_i, x_{i+1}) for $1 \leq i \leq n-1$ as illustrated in Figure 4.

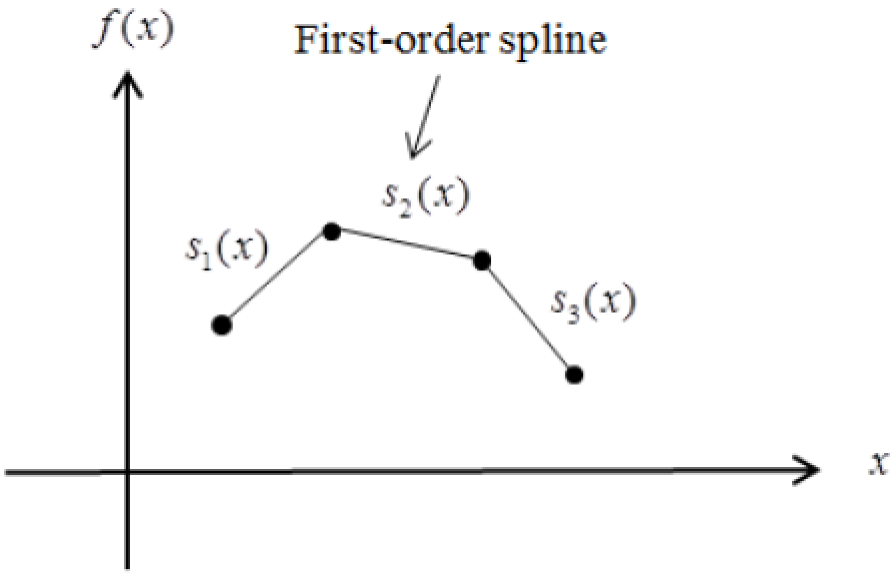


Figure 4: Graph of first-order spline.

LINEAR SPLINE (Cont.)

Linear Spline: Formula

For linear spline, the set of straight line functions for n given points and $n-1$ intervals are

$$s_1(x) = f_1 + \frac{f_2 - f_1}{x_2 - x_1}(x - x_1) \qquad x_1 \le x \le x_2$$

$$s_2(x) = f_2 + \frac{f_3 - f_2}{x_3 - x_2}(x - x_2) \qquad x_2 \le x \le x_3$$

$$s_3(x) = f_3 + \frac{f_4 - f_3}{x_4 - x_3}(x - x_3) \qquad x_3 \le x \le x_4$$

LINEAR SPLINE (Cont.)

Example 5

Consider the following data.

x	2	5	8	11
$f(x)$	1.5	4	2.8	6

i) Derive a set of linear functions for the data given.
ii) Evaluate the function at $x = 6.5$.

LINEAR SPLINE (Cont.)

Solution

i) Since we have four data, so we can determine three splines function,

$$s_1(x) = f_1 + \frac{f_2 - f_1}{x_2 - x_1}(x - x_1) = 1.5 + \frac{4.0 - 1.5}{5.0 - 2.0}(x - 2.0) \qquad 2.0 \le x \le 5.0$$

$$s_2(x) = f_2 + \frac{f_3 - f_2}{x_3 - x_2}(x - x_2) = 4.0 + \frac{2.8 - 4.0}{8.0 - 5.0}(x - 5.0) \qquad 5.0 \le x \le 8.0$$

$$s_3(x) = f_3 + \frac{f_4 - f_3}{x_4 - x_3}(x - x_3) = 2.8 + \frac{6.0 - 2.8}{11.0 - 8.0}(x - 8.0) \qquad 8.0 \le x \le 11.0$$

ii) Since $x = 6.5$ lies in the second interval, so we will use s_2 to make the prediction,

$$s_2(6.5) = 4.0 + \frac{2.8 - 4.0}{8.0 - 5.0}(6.5 - 5.0) = 3.4$$

QUADRATIC SPLINE

Introduction

In the second-order spline, we are ending the quadratic equations connecting each pair of interval (x_i, x_{i+1}) for $1 \leq i \leq n-1$ as illustrated in Figure 5.

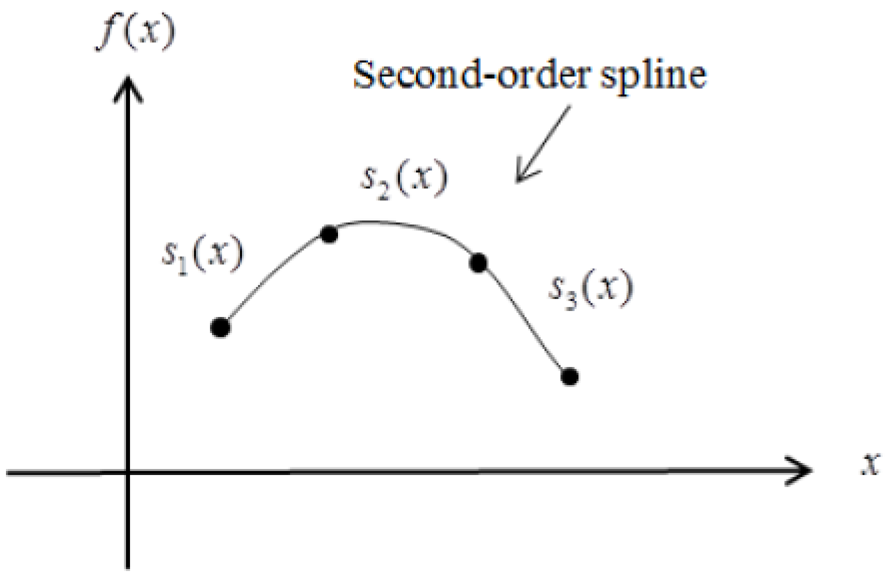


Figure 5: Graph of second-order spline.

QUADRATIC SPLINE (Cont.)

Quadratic Spline: Formula

In general the quadratic spline function is:

$$s_i(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 \qquad x_i \le x \le x_{i+1}$$

where the constants a, b and c can be calculated using

$$a_i = f_i$$

$$f_{i+1} = f_i + b_i h_i + c_i h_i^2$$

$$b_{i+1} = b_i + 2c_i h_i$$

and given that $c_1 = 0$ and $h_i = x_{i+1} - x_i$.

QUADRATIC SPLINE (Cont.)

Example 7

Consider the following data.

x	2	2.5	3	3.5
$f(x)$	0.125	0.064	0.037	0.0233

i) Fit the data with second-order splines.
ii) Evaluate the function at $x = 2.2$ and $x = 3.3$.

QUADRATIC SPLINE (Cont.)

Solution

i) Find $s_1(x)$ for interval $2 \leq x \leq 2.5$:

$$s_1(x) = a_1 + b_1(x - x_1) + c_1(x - x_1)^2$$

$$c_1 = 0, a_1 = f_1 = 0.125$$

$$s_1(x) = 0.125 + b_1(x - 2)$$

$$h_1 = x_2 - x_1 \rightarrow 2.5 - 2 = 0.5$$

$$f_1 + b_1 h_1 + c_1 h_1^2 = f_2$$

$$0.125 + b_1(0.5) = 0.064 \rightarrow b_1 = -0.122$$

$$b_1 + 2c_1 h_1 = b_2 \rightarrow b_2 = -0.122$$

Thus,

$$s_1(x) = 0.125 - 0.122(x - 2).$$

QUADRATIC SPLINE (Cont.)

Solution (Cont.)

Find $s_2(x)$ for interval $2.5 \le x \le 3.0$:

$$s_2(x) = a_2 + b_2(x - x_2) + c_2(x - x_2)^2$$

$$a_2 = f_2 = 0.064$$

$$s_2(x) = 0.064 + b_2(x - x_2) + c_2(x - x_2)^2$$

$$h_2 = x_3 - x_2 \rightarrow 3 - 2.5 = 0.5$$

$$f_2 + b_2 h_2 + c_2 h_2^{\;2} = f_3$$

$$0.064 + (-0.122)(0.5) + c_2(0.5)^2 = 0.0370 \rightarrow c_2 = 0.136$$

$$b_2 + 2c_2 h_2 = b_3$$

$$(-0.122) + 2(0.136)(0.5) = b_3 \rightarrow b_3 = 0.014$$

Thus,

$$s_2(x) = 0.064 - 0.122(x - 2.5) - 0.136(x - 2.5)^2$$

QUADRATIC SPLINE (Cont.)

Solution (Cont.)

Find $s_3(x)$ for interval $3 \leq x \leq 3.5$:

$$s_3(x) = a_3 + b_3(x - x_3) + c_3(x - x_3)^2$$

$$a_3 = f_3 = 0.0370$$

$$s_3(x) = 0.037 + b_3(x - x_3) + c_3(x - x_3)^2$$

$$h_3 = x_4 - x_3 \rightarrow 3.5 - 3 = 0.5$$

$$f_3 + b_3 h_3 + c_3 {h_3}^2 = f_4$$

$$0.037 + (0.014)(0.5) + c_2(0.5)^2 = 0.0233 \rightarrow c_3 = -0.0828$$

Thus,

$$s_3(x) = 0.037 + 0.014(x - 3) - 0.0828(x - 3)^2$$

QUADRATIC SPLINE (Cont.)

Solution

Therefore:

$$s_1(x) = 0.125 - 0.122(x-2) \qquad 2.0 \le x \le 2.5$$

$$s_2(x) = 0.064 - 0.122(x-2.5) - 0.136(x-2.5)^2 \qquad 2.5 \le x \le 3.0$$

$$s_3\left(x\right) = 0.037 + 0.014(x-3) - 0.0828(x-3)^2 \qquad 3.0 \le x \le 3.5$$

ii) To estimate the value of $f\ (x)$ at $x\ =\ 2.2$, we use $s_1(x)$ since $x\ =\ 2.2$ lies in the interval $[2,2.5]$. Hence,

$$s_1(2.2) = 0.125 - 0.122(2.2-2) = 0.1006$$

To estimate the value of $f\ (x)$ at $x\ =\ 3.3$, we use $s_1(x)$ since $x\ =\ 3.3$ lies in the interval $[3,3.5]$. Hence,

$$s_3\left(3.3\right) = 0.037 + 0.014(3.3-3) - 0.0828(3.3-3)^2 = 0.0337$$

CONCLUSION

- Interpolation method is used to estimate the value of $f(x)$ for any value of x within the range of discrete data set of known data points .
- The methods involve in this chapter are **polynomial interpolation method** and **splines method**.
- Polynomial interpolation method covers in this chapter are **Newton interpolation method** and **Lagrange interpolation method** while splines method divided into two methods which are **linear spline** and **quadratic spline**.
- Inverse interpolation method is to estimate the value of x for any value of $f(x)$ within the range of discrete data set of known data points .

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