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The Study of the Curves of Functions for Data Points

Hla Myint Kyaw

Abstract

The unknown functions for data points are studied. We need to obtain the physically correct results. A cubic spline routine was developed for equally and unequally spaced sequential data points. Cubic spline theory is reviewed. A visual basic computer program in Excel (2003) was created to fit a spline to input data points. Therefore, the graphs of approximating functions are discussed.

Key words: Spline, Interpolation, Curves, Functions, Curve fitting, Cubic

Introduction

There are two topics to be dealt with in this research paper, namely, interpolation and curve fitting (data fitting). The objective is to fit a cubic spline to data points. This paper will develop the governing equations for a cubic spline. Lagrange's interpolation and cubic spline interpolation are compared with their graphs for data points. Finally, conclusions will be discussed.

Interpolation

Interpolation is to connect discrete data points in a plausible way so that one can get reasonable estimates of data points between the given points. Interpolation methods can be divided into main categories.

Curve Fitting

Curve fitting, on the other hand, is to find a curve that could best indicate the trend of a given set of data. The curve does not have to go through the data points.

Spline

A spline is a kind of template that architects use to draw a smooth curve between two points. That is why we often resort to the piecewise-cubic curve constructed by the individual third degree polynomials assigned to each subinterval, which is called the cubic spline interpolation. Splines are interpolative polynomials that involve information concerning the

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derivative of the function at certain points. While one can construct splines of any order, the most common ones are cubic splines as they generate tri-diagonal equations for the coefficients of the polynomials. Cubic is an equation of degree three or less.

Materials and Methods

Lagrange's Interpolation

For a given set of (N+1) data points $\{(X_0,Y_0),---,(X_N,Y_N)\}$, we want to find the coefficients of an Nth-degree polynomial function to match them:

$$P_N(x) = a_0 + a_1x + a_2x^2 + --- + a_Nx^N$$

$$a_0 + a_1x_0 + a_2x_0^2 + --- + a_Nx_0^N = y_0$$

$$a_0 + a_1x_1 + a_2x_1^2 + --- + a_Nx_1^N = y_1$$

$$a_0 + a_1x_2 + a_2x_2^2 + --- + a_Nx_2^N = y_2$$

$$a_0 + a_1x_N + a_2x_N^2 + --- + a_Nx_N^N = y_N$$

Interpolation by Cubic Spline

For a given set of data points $\{(x_k, y_k), k = 0 : N\}$, the cubic spline s(x) consists of N cubic polynomial $s_k(x)$'s assigned to each subinterval satisfying the following constraints (S0) - (S4).

(S0) $s(x) = S_k(x) = S_{k,3}(x-x_k)^3 + S_{k,2}(x-x_k)^2 + S_{k,1}(x-x_k) + S_{k,0}$ for $x \in [x_k, x_{k+1}]$, $k = 0 : N$

(S1) $s_k(x_k) = S_{k,0} = y_k$ for $k = 0 : N$

(S2) $s_{k-1}(x_k) \equiv s_k(x_k) = S_{k,0} = y_k$ for $k = 1 : N-1$

(S3) $s'_{k-1}(x_k) \equiv s'_k(x_k) = S_{k,1}$ for $k = 1 : N-1$

(S4) $s''_{k-1}(x_k) \equiv s''_k(x_k) = 2S_{k,2}$ for $k = 1 : N-1$

These constraints (S1) - (S4) amount to a set of $N+1+3(N-1) = 4N-2$ linear equations having 4N coefficients of the N cubic polynomials

$$\{S_{k,0}, S_{k,1}, S_{k,2}, S_{k,3}, k = 0 : N-1\}$$

as their unknowns. Two additional equations necessary for the equations to be solvable are support to come from the boundary conditions for the first/ second-order derivatives at the end points (x_0,y_0) and (x_N,y_N) as listed in Table 1.

Table 1. Boundary Conditions for a Cubic Spline

(i)	First-order derivatives specified	$s'_0(x_0) = S_{0,1},\ s'_N(x_N) = S_{N,1}$
(ii)	Second-order derivatives specified (end-curvature adjusted)	$s''_0(x_0) = 2S_{0,2},\ s''_N(x_N) = 2S_{N,2}$
(iii)	Second-order derivatives extrapolated	$s''_0(x_0) \equiv s''_1(x_1) + \frac{h_0}{h_1}(s''_1(x_1) - s''_2(x_2))$ $s''_N(x_N) \equiv s''_{N-1}(x_{N-1}) + \frac{h_{N-1}}{h_{N-2}}(s''_{N-1}(x_{N-1}) - s''_{N-2}(x_{N-2}))$

Now, noting from (S1) that $S_{k,0} = y_k$, we will arrange the constraints (S2)-(S4) and eliminate $S_{k,1}$, $S_{k,3}$'s to set up a set of equations with respect to the N+1 unknowns $\{S_{k,2},\ k=0 : N\}$. In order to do so, we denote each interval width by $h_k = x_{k+1} - x_k$ and substitute (S0) into (S4) to write

$$s''_k(x_{k+1}) = 6S_{k,3}\, h_k + 2S_{k,2} \equiv s''_{k+1}(x_{k+1}) = 2S_{k+1,2}$$

$$S_{k,3}\, h_k = \frac{1}{3}(S_{k+1,2} - S_{k,2}) \tag{1,a}$$

$$S_{k-1,3}\, h_{k-1} = \frac{1}{3}(S_{k,2} - S_{k-1,2}) \tag{1,b}$$

We substitute these equations into (S2) with (k+1) in place of k.

$$S_k(x_{k+1}) = S_{k,3}(x_{k+1}-x_k)^3 + S_{k,2}(x_{k+1}-x_k)^2 + S_{k,1}(x_{k+1}-x_k) + S_{k,0} \equiv y_{k+1}$$

$$S_{k,3}h_k^3 + S_{k,2}h_k^2 + S_{k,1}h_k + y_k \equiv y_{k+1}$$

to eliminate $S_{k,3}$'s and rewrite it as

$$\frac{h_k}{3}(S_{k+1,2} - S_{k,2}) + S_{k,2}h_k + S_{k,1} = \frac{y_{k+1} - y_k}{h_k} = dy_k$$

$$h_k(S_{k+1,2} + 2S_{k,2}) + 3S_{k,1} = 3\ dy_k \tag{2,a}$$

$$h_{k-1}(S_{k,2} + 2S_{k-1,2}) + 3S_{k-1,1} = 3\ dy_{k-1} \tag{2,b}$$

We also substitute Eq. (1,b) into (S3)

$$s'_{k-1}(x_k) = 3S_{k-1,3}h_{k-1}^2 + 2S_{k-1,2}h_{k-1} + S_{k-1,1} \equiv s'_k(x_k) = S_{k,1}$$

to write

$$S_{k,1} - S_{k-1,1} = h_{k-1}(S_{k,2} - S_{k-1,2}) + 2h_{k-1}S_{k-1,2} = h_{k-1}(S_{k,2} + S_{k-1,2}) \tag{3}$$

In order to use this for eliminating $S_{k,1}$ from Eq.(2), we subtract (2,b) from (2,a) to write

$$h_k(S_{k+1,2} + 2S_{k,2}) - h_{k-1}(S_{k,2} + 2S_{k-1,2}) + 3(S_{k,1} - S_{k-1,1}) = 3\ (dy_k - dy_{k-1})$$

and then substitute Eq. (3) into this to write

$$h_k(S_{k+1,2} + 2S_{k,2}) - h_{k-1}(S_{k,2} + 2S_{k-1,2}) + 3h_{k-1}(S_{k,2} + S_{k-1,2}) = 3\ (dy_k - dy_{k-1})$$

$$h_{k-1}S_{k-!,2} + 2(h_{k-1} + h_k)\ S_{k,2} + h_k\ S_{k+1,2} = 3\ (dy_k - dy_{k-1}) \tag{4}$$

for $k = 1 : N-1$

Since these are N-1 equations with respect to N+1 unknowns $\{S_{k,2},\ k = 0 : N\}$, we need to more equations from the boundary conditions to be given as listed in Table 1.

How do we convert the boundary condition into equations? In the case where the first-order derivatives on the two boundary points are given as (i) in Table 1, we write Eq. (2,a) for $k = 0$ as

$$h_0(S_{1,2} + 2S_{0,2}) + 3S_{0,1} = 3dy_0,$$

$$2h_0\ S_{0,2} + h_0S_{1,2} = 3(dy_0 - S_{0,1}) \tag{5,a}$$

We also write Eq. (2,b) for $k = N$ as

$$h_{N-1}(S_{N,2} + 2S_{N-1,2}) + 3(S_{N-1,1}) = 3dy_{N-1}$$

and substitute Eq.(3) (k=N) into this to write

$$h_{N-1}S_{N-1,2} + 2h_{N-1}S_{N,2} = 3(S_{N,1} - dy_{N-1}) \tag{5,b}$$

Equations (5,a) and (5,b) are two additional equations that we need to solve Eq.(4) and that's it. In the case where the second-order derivatives on the two boundary points are given as (ii) in Table 1, $S_{0,2}$ and $S_{N,2}$ are directly known from the boundary conditions as

$$S_{0,2} = \frac{1}{2} s''_0(x_0),\ S_{N,2} = \frac{1}{2} s''_N(x_N) \tag{6}$$

and, subsequently, we have just N-1 unknowns. In the case where the second-order derivatives on the two boundary points are given as (iii) in Table 1.

$$s''_0(x_0) \equiv s''_1(x_1) + \frac{h_0}{h_1}(s''_1(x_1)-s''_2(x_2))$$

$$s''_N(x_N) \equiv s''_{N-1}(x_{N-1}) + \frac{h_{N-1}}{h_{N-2}}(s''_{N-1}(x_{N-1})-s''_{N-2}(x_{N-2}))$$

We can instantly convert these into two equations with respect to $S_{0,2}$ and $S_{N,2}$ as

$$h_1 S_{0,2} - (h_0+h_1)\, S_{1,2} + h_0\, S_{2,2} = 0 \tag{7,a}$$

$$h_{N-2} S_{N,2} - (h_{N-1}+h_{N-2})\, S_{N-1,2} + h_{N-1}\, S_{N-2,2} = 0 \tag{7,b}$$

Finally, we combine the two equations (5,a) and (5,b) with Eq.(4) to write it in the matrix-vector form as

$$\begin{pmatrix} 2h_0 & h_0 & 0 & 0 & 0 \\ h_0 & 2(h_0+h_1) & h_1 & 0 & 0 \\ 0 & \bullet & \bullet & \bullet & 0 \\ 0 & 0 & h_{N-2} & 2(h_{N-2}+h_{N-1}) & h_{N-1} \\ 0 & 0 & 0 & h_{N-1} & 2h_{N-1} \end{pmatrix} \begin{pmatrix} S_{0,2} \\ S_{1,2} \\ \bullet \\ S_{N-1,2} \\ S_{N,2} \end{pmatrix} = \begin{pmatrix} 3(dy_0-S_{0,1}) \\ 3(dy_1-dy_0) \\ \bullet \\ 3(dy_{N-1}-dy_{N-2}) \\ 3(S_{N,1}-dy_{N-1}) \end{pmatrix} \tag{8}$$

After solving this system of equation for $\{S_{k,2},\ k = 0 : N\}$, we substitute them into (S1), Eq.(2), and Eq.(1) to get the other coefficients of the cubic spline as

$$S_{k,0} \overset{S1}{=} y_k,\ S_{k,1} \overset{Eq(2)}{=} dy_k - \frac{h_k}{3}(S_{k+1,2} + 2S_{k,2})$$

$$S_{k,3} \overset{Eq(1)}{=} \frac{S_{k+1,2} - S_{k,2}}{3h_k}$$

Remark:

There are some popular types of splines:

(1) Natural splines (Lemma)

$s''_0(x_0) = s''_N(x_N) = 0$

(2) Parabolic run-out splines

$s''_0(x_0) = s''_0(x_1)$

$s''_N(x_N) = s''_{N-1}(x_{N-1})$

(3) Clamped splines (Lemma)

$s'_0(x_0) = s'(x_0)$

$s'_N(x_N) = s'(x_N)$

(4) Extrapolated splines

$$s''_0(x_0) \equiv s''_1(x_1) + \frac{h_0}{h_1}(s''_1(x_1) - s''_2(x_2))$$

$$s''_N(x_N) \equiv s''_{N-1}(x_{N-1}) + \frac{h_{N-1}}{h_{N-2}}(s''_{N-1}(x_{N-1}) - s''_{N-2}(x_{N-2}))$$

(5) Periodic cubic splines

$s(x_0) = s(x_N)$

$s'(x_0) = s'(x_N)$

$s''(x_0) = s''(x_N)$

Shape-Preserving Piecewise Cubic Hermite Interpolation

Many of the most effective interpolation techniques are based on piecewise cubic polynomials. Let h_k denote the length of the kth subintervals:

$h_k = x_{k+1} - x_k$

Then the first divided difference, δ_k, is given by

$$\delta_k = \frac{y_{k+1} - y_k}{h_k}$$

Let d_k denote the slope of the interpolant at x_k:

$d_k = P'(x_k)$

For the piecewise linear interpolant, $d_k = \delta_{k-1}$ or δ_k, but this is not necessarily true for higher order interpolants.

Consider the following function on the interval $x_k \le x \le x_{k+1}$, expressed in terms of local variables $s = x - x_k$ and $h = h_k$:

$$P(x) = \frac{3hs^2 - 2s^3}{h^3} y_{k+1} + \frac{h^3 - 3hs^2 + 2s^3}{h^3} y_k + \frac{s^2(s-h)}{h^2} d_{k+1} + \frac{s(s-h)^2}{h^2} d_k$$

This is a cubic polynomial in s, and hence in x, that satisfies four interpolation conditions, two on function values and two on the possibly unknown derivative values:

$P(x_k) = y_k$, $P(x_{k+1}) = y_{k+1}$,

$P'(x_k) = d_k$, $P'(x_{k+1}) = d_{k+1}$,

Functions that satisfy interpolation conditions on derivatives are known as Hermite or osculatory interpolants, because of the higher order contact at the interpolation sites. ("Osculari" means "to kiss" in Latin).

If we happen to know both function values and first derivative values at a set of data points, then piecewise cubic Hermite interpolation can reproduce those data. But if we are not given the derivative values, we need to define the slopes d_k somehow. Of the many possible ways to do this, we will describe two, which MATLAB calls pchip and spline.

The acronym pchip abbreviates "piecewise cubic Hermite interpolating polynomial". Although it is fun to say, the name does not specify which of the many possible interpolants is actually being used. In fact, spline interpolants are also piecewise cubic Hermite interpolating polynomials, but with different slopes. Our particular pchip is a shape-preserving, "visually pleasing" interpolant. Fig. 4 shows how pchip interpolates our sample data.

The key idea is to determine the slopes d_k so that the function values do not overshoot the data values, at least locally. If δ_k and δ_{k-1} have opposite signs or if either of them is zero, then x_k is a discrete local minimum or maximum, so we set

$d_k = 0$

This is illustrated in the Fig. 4. The shape-preserving interpolant is formed from two different cubics. The two cubics interpolate the center value and their derivatives are both zero there. But there is a jump in the second derivative at the breakpoint. The breakpoints of a spline are also referred to as its knots.

If δ_k and δ_{k-1} have the same sign and the two intervals have the same length, then d_k is taken to be the harmonic mean of the two discrete slopes:

$$\frac{1}{d_k}=\frac{1}{2}\left(\frac{1}{\delta_{k-1}}+\frac{1}{\delta_k}\right)$$

In other words, at the breakpoint, the reciprocal slope of the Hermite interpolant is the average of the reciprocal slopes of the piecewise linear interpolant on either side.

If δ_k and δ_{k-1} have the same sign, but the two intervals have different lengths, then d_k is a weighted harmonic mean, with weights determined by the lengths of the two intervals:

$$\frac{w_1+w_2}{d_k}=\frac{w_1}{\delta_{k-1}}+\frac{w_2}{\delta_k})$$

where

$w_1 = 2h_k + h_{k-1}$, $w_2 = h_k + 2h_{k-1}$

This defines the pchip slopes at interior breakpoints, but the slopes d_1 and d_N at either end of the data interval are determined by a slightly different, one-sided analysis. The details are in pchiptx.m. It is described as follows:

The idea is to use a single cubic on the first two intervals, $x_1 \le x \le x_3$ and on the last two subintervals, $x_{N-2} \le x \le x_N$. In effect, x_2 and x_{N-1} are knots. If the knots are equally spaced with all $h_k = 1$, this leads to,

$$d_1+2d_2=\frac{5}{2}\delta_1+\frac{1}{2}\delta_2$$

$$2d_{N-1}+d_N=\frac{1}{2}\delta_{N-2}+\frac{5}{2}\delta_{N-1}$$

The details if the spacing is not equal to one are in splinetx.m. This leads to the condition.

$$h_k d_{k-1} + 2(h_{k-1}+h_k)d_k + h_{k-1}d_{k+1} = 3(h_k\delta_{k-1}+h_{k-1}\delta_k)$$

If the knots are equally spaced, so that h_k does not depend on k, this becomes

$$d_{k-1}+4d_k+d_{k+1} = 3\delta_{k-1}+3\delta_k$$

Comparison of Lagrange's and Cubic Spline Interpolations

We will consider the data points {(-4,16),(-3,9),(-2,4),(-1,1),(0,0),(1,1), (2,4),(3,9),(4,16)}if $y(x)=x^2$. The values and graphs of approximating functions are compared as follows:

Table 2. Comparison of the two methods

X	Y (ACTUAL)	Y (LAG)	Y (CLAMPED SPLINE)
-4	16	16	16
-3.95	15.6025	15.6025	15.6025
-3.9	15.21	15.21	15.21
-3.85	14.8225	14.8225	14.8225
-3.8	14.44	14.44	14.44
-3.75	14.0625	14.0625	14.0625
-3.7	13.69	13.69	13.69
-3.65	13.3225	13.3225	13.3225
-3.6	12.96	12.96	12.96
-3.55	12.6025	12.6025	12.6025
-3.5	12.25	12.25	12.25

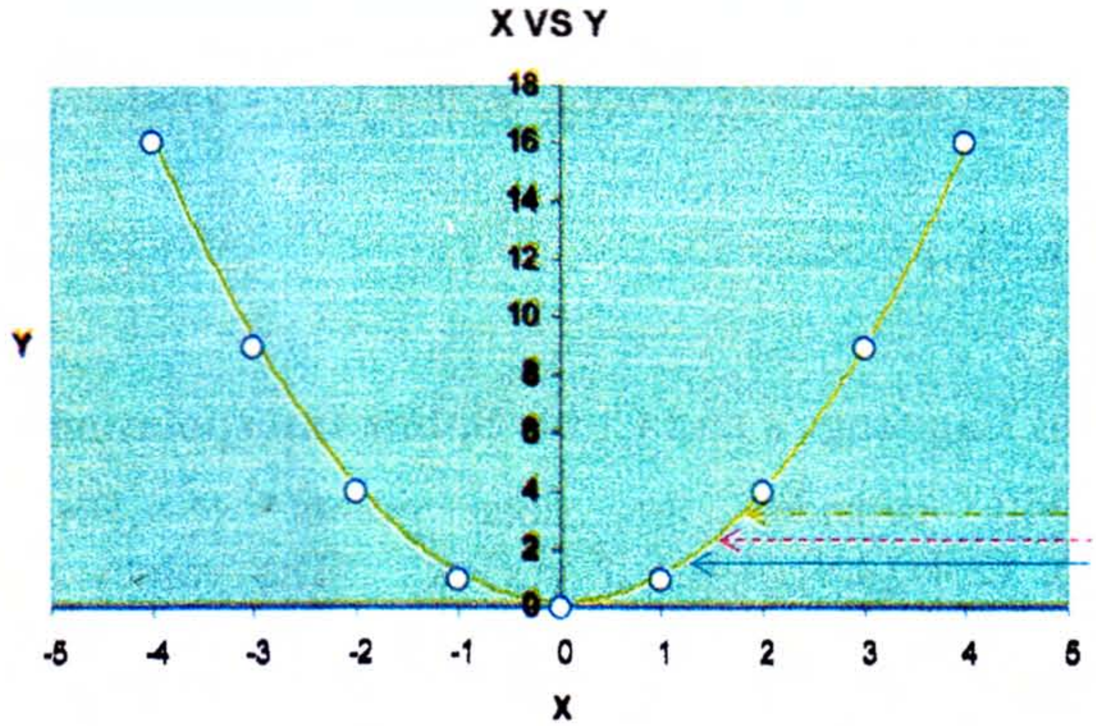

Fig. 1. The graphs of functions of the two methods
represents actual function
represents Lagrange's interpolation function
represents cubic clamped spline interpolation function

Let us consider the data points $\{(-1,4),(-\frac{1}{2},1),(\frac{1}{2},1),(1,4)\}$ if $y=4x^2$.

The graphs of approximating functions are compared as follows:

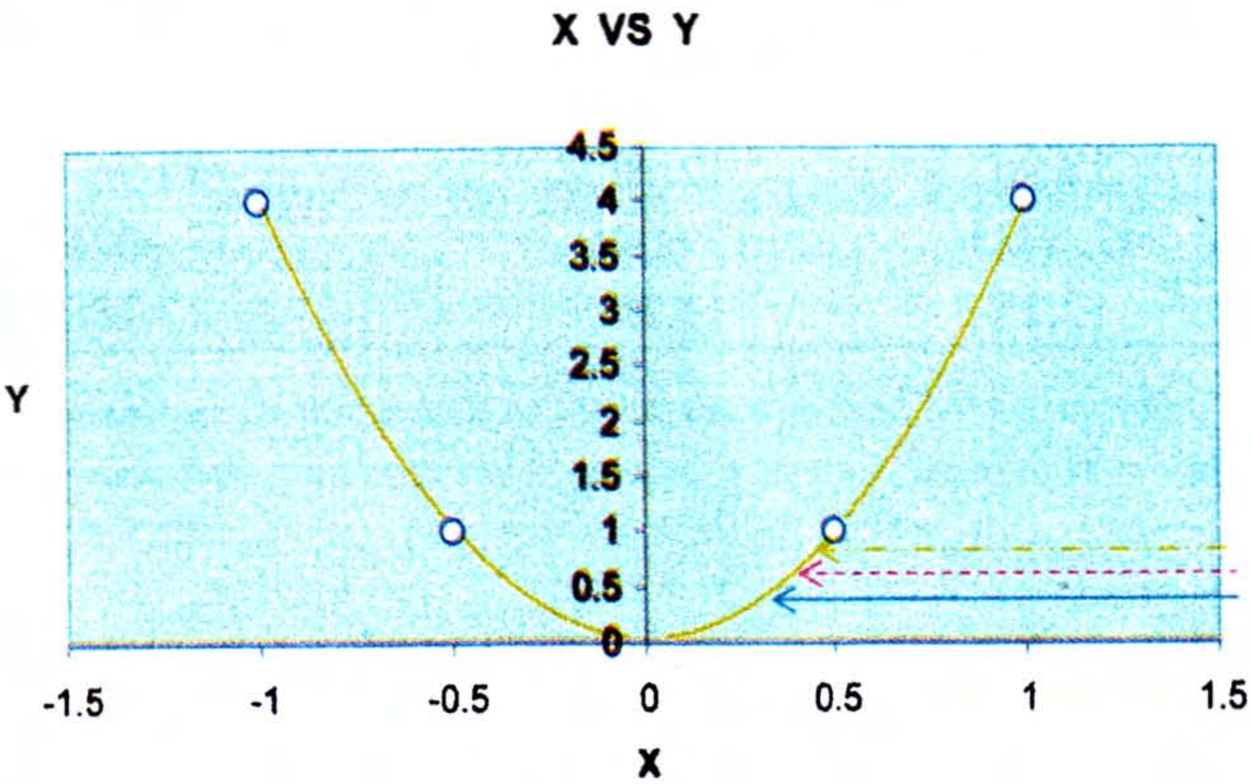

Fig. 2. The graphs of functions of two methods
represents actual function
represents Lagrange's interpolation function
represents cubic clamped spline interpolation function

Next, let us consider the data points $\{(-1,1),(0,0),(1,1)\}$ if $y = x^4$.

Next, let us consider the data points {(-1,1),(0,0),(1,1)} if $y = x^4$. The graphs of approximating functions are compared as follows:

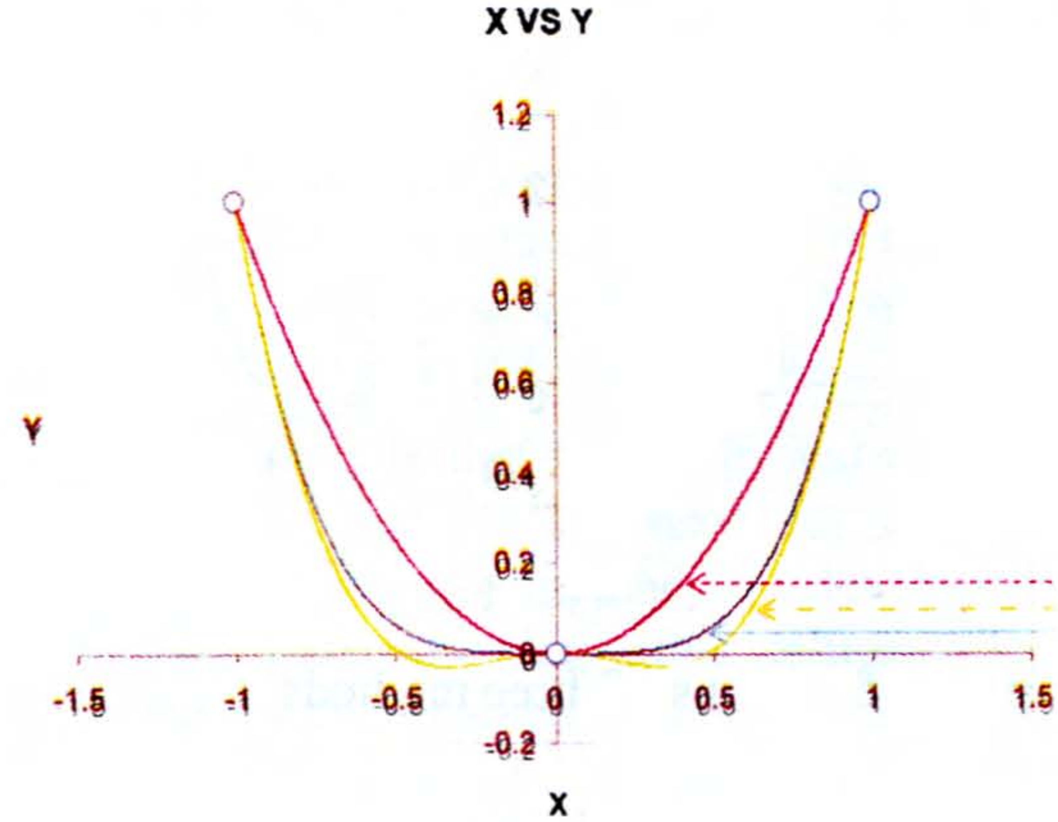

Fig. 3. The graphs of functions of two methods
represents actual function
represents Lagrange's interpolation function
represents cubic clamped spline interpolation function

Comparison of Lagrange's, Extrapolated Cubic Spline and Shape-Preserving Piecewise Cubic Hermite Interpolations

We will consider the data points

{(-2,0),(-1,0),(-0.5,0.25),(0,1),(0.5,0.25),(1,0),(2,0)}. The values and graphs of approximating functions are compared as follows:

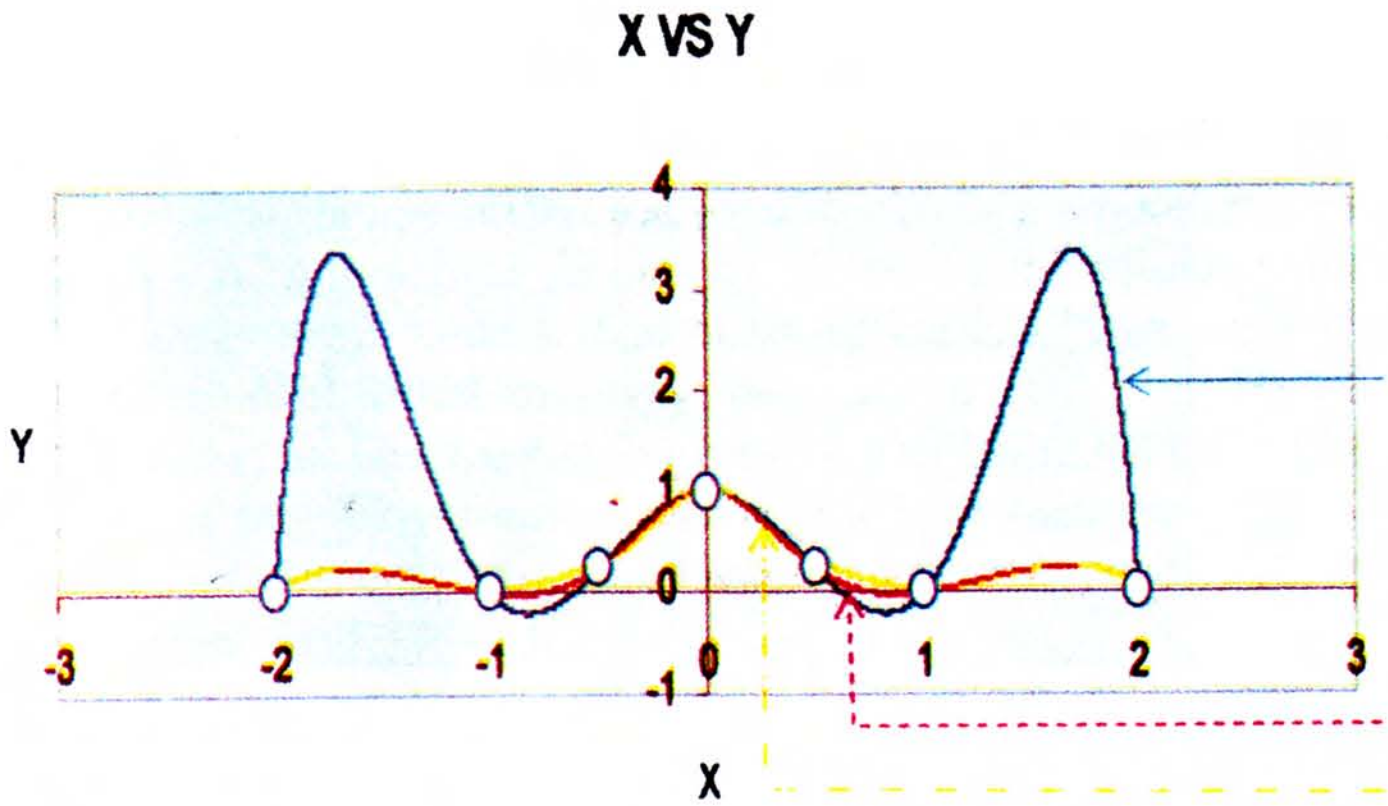

Fig. 4. The graphs of functions of three methods
represents Lagrange's interpolation function
represents extrapolated cubic spline interpolation function
represents shape-preserving piecewise Hermite interpolation function

Results and Discussion

With the actual functions, Lagrange's and the clamped cubic spline interpolation functions are compared from Fig. 1, Fig. 2 and Fig. 3. We can see that the pattern of the graph of Lagrange's function is identical with that of the clamped cubic spline function from Fig. 1 and Fig. 2. The graphs of their functions coincide with the graph of the actual function. But as shown in Fig. 3, the graphs of their functions do not coincide with the graph of the actual function. The graph of spline function is closer to that of the actual function than Lagrange's function.

Interpolation is used to estimate the value of a function between known data points without knowing the actual function. Therefore Lagrange's and extrapolated cubic spline and shape-preserving piecewise cubic Hermite spline interpolations are used to obtain a smoother curve as shown in Fig. 4. A practical feature of splines is the minimum of the oscillating behavior they possess. The cubic spline has "less wiggle". Splines are smooth and continuous across the interval. To obtain a smoother curve, cubic splines are frequently recommended.

Conclusion

A cubic spline curve fit routine was successfully implemented. The results show that the cubic spline provides an adequate curve fit for most data sets. Because the cubic spline method involves connecting individual segments, the cubic spline avoids oscillation problems in the curve fit. Overall, the cubic spline provides a good curve fit for arbitrary data points. Splines are highly useful tools for numerical data analysis. Splines can be made to fit even the most random of data, making numerical analysis possible even when the actual function is not known.

Finally, we can conclude that the pchip and the cubic spline have low curvature. The cubic splines are used for chemical engineering applications. In 1993, a cubic spline method was developed for finding the periodicity of stellar light curves using cubic splines. The experimental results are closer to the results obtained from cubic splines. Consequently, shape of our hand can be preserved by the method of shape-preserving piecewise cubic Hermite interpolation polynomial. In addition, pchip is guaranteed to preserve shape, but the spline might not.

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