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The Use of Piecewise Polynomial Interpolation in Chemical Engineering

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Abstract: This paper gives an application of spline interpolation to study chemical engineering problem. The various degree of piecewise polynomial used separately. Chemical engineering problem represented in the form of the data points for which the various piecewise polynomials are as interpolating polynomial. The objective of this paper is to check the smoothness of curve fitting. Results are presented in tabular and graphical forms are quite encouraged for the further use of spline Interpolation.

Keywords: Interpolation, Linear spline, Quadratic spline, Cubic spline, Cubic Hermite spline, MATLAB.

1. Introduction

In this paper we discuss about piecewise polynomial interpolation methods to solve large data problem in chemical engineering by curve fitting and which interpolation method is best for us.

In practical fields such as engineering, medicine, physics, agriculture and computer graphics the amount of data obtained through experimental or statistical surveys is usually very large. The use of an interpolation scheme for the construction of spline curves from the given data consisting of a relatively large number of points will yield a huge number of curve segments. On the other hand, in most applications the points are subject to measurement errors. We can hope that with the curve approximation, these errors will be smoothed out and the resulting curve will look smooth enough.

Before the inventing of calculators mathematical tables were a necessity for everybody applying mathematics. Interpolation was first used to calculate additional values based on tabulated values of special functions.

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The approximation theory is one of the main topics of numerical analysis. It is a foundation for numeral algorithms in the different fields of applied mathematics. Polynomial interpolation is especially important, since it offers an approximating function in a closed form, which is widely used in implementations. Polynomials are the most easily handled in practice, since they can be represented by restricted information, evaluated in limited number of basic operations and easily integrated or differentiated.

In recent years, splines have attracted attention of both researchers and users who need various approximation tools. To sum up, linear splines are a set of joint line segments, a continuous function with discontinuous first derivative at the knots. Quadratic splines have a continuous first derivative, cubic splines continuous first and second derivatives, and so on. Linear splines are evidently too rough of an approximation to a physical spline, a cubic spline is adequate, quartic and higher order splines are possible but require more computation[1].

2. Spline Interpolation

Interpolation is an estimation of a value within two known values. It is an estimation of an unknown quantity between two known quantities or drawing conclusions about missing information from the available one. Interpolation is useful where the data surrounding missing data is available and where longer term cycles are known. Interpolation is a method of building a function that crosses through a discrete set of known data points.
There are many different interpolation methods (four of them are discussed below and compared them). While choosing an appropriate algorithm and interpolation method some of the concerns should be foreseen, for example how accurate is the method, how smooth is the interpolate or how many data points are needed and etc.

2.1 Linear Interpolation:

Linear interpolation has been used for filling the gaps in tables, often with astronomical data. It is believed that it was used by Babylonian astronomers, by mathematicians in Seleucid Mesopotamia and by the Greek astronomer and mathematician, Hipparchus. A description of linear interpolation can also be found in the Almagest by Ptolemy.

The linear splines are much simpler than cubic splines. The result of linear interpolation is a set of straight lines connecting the data points. For two spatial dimensions, the extension of linear interpolation is called bilinear interpolation. In three dimensions it is called tri-linear interpolation[2].

This method is often used in chemical engineering since the resulting spline never overshoots. Even so, when a smooth interpolate is desired, a higher order spline is needed. Linear spline models are criticized because of the abrupt change in trend going from one segment to the next, which does not represent what would naturally occur. The true change in trend should be smooth. In mathematical terms this means that the fitting function should have a continuous derivative a teach value of the independent variable. This is not possible for linear splines, but it is possible for quadratic splines that are joined segments of parabolas[3].

2.2 Quadratic Spline Interpolation:

A quadratic spline interpolation method produces a better fit to a continuous function than a linear spline does. A quadratic spline is a continuously differentiable piecewise quadratic function, where quadratic includes all linear combinations of the basic monomials. Quadratic splines are not used in applications as much as natural cubic splines. However, the derivations of interpolating quadratic and cubic splines are similar enough, so that an understanding of the simpler second-degree spline theory allows us to grasp easily the more complicated third-degree spline theory[3].

2.3 Cubic Spline Interpolation:

Cubic splines play an important role in fields where smooth interpolation is essential in modeling, for example, animation and image scaling. In computer graphics interpolating cubic splines are often used to define smooth motion of objects and cameras passing through user-specified positions in a key frame animation system. In image processing splines prove useful in implementing high-quality image magnification.

2.4 Cubic Hermite Spline Interpolation:

There are many kinds of piecewise polynomial interpolation. We can try to modify a set of cubic splines with a set of other polynomials such as the cubic Hermite polynomials.

These cubic Hermite polynomials allow us to provide not only continuity of the first order derivatives of the curve but also to match the set of chosen slopes. This interpolation is appropriate when both the function and the derivative values are available .In the mathematical field of numerical analysis a cubic Hermite spline, named after Charles Hermite, is a third-degree spline in Hermite form. The Hermite form has two control points and two control tangents for each polynomial. They are simple to calculate but at the same time too powerful[4].

3. Application

3.1 Experimental Results in Chemical Engineering:

The Results of experiments with different flow rates vs. pump power are given below where we use Linear, Quadratic, Cubic and Cubic Hermite Spline interpolation techniques to fit the data.

Spray Dryer Data is given in the Table below. The table shows the results of grape seed extract for different pump power and flow rate values[5].

Table 1: Pump Power vs. Flow Rate

Pump Power	T (min)	Flow Rate (ml/min)
0	0	0
10	1014	493
20	625	800
30	437	1144
40	347	1441
50	244	2049
60	236	2119
70	209	2392
80	155	3226
90	144	3472
100	141	3546

For the values in the table containing experimental data, different spline interpolation methods are demonstrated. For specific type of data, we observed and discussed advantages and disadvantages of different methods. Linear spline interpolation method was used to fit the data in MATLAB. As shown in Figure 1, linear spline has hardly any smoothness. It preserves the local monotonicity of the data and never overshoots. That is why it is widely used and very famous in chemical engineering applications.

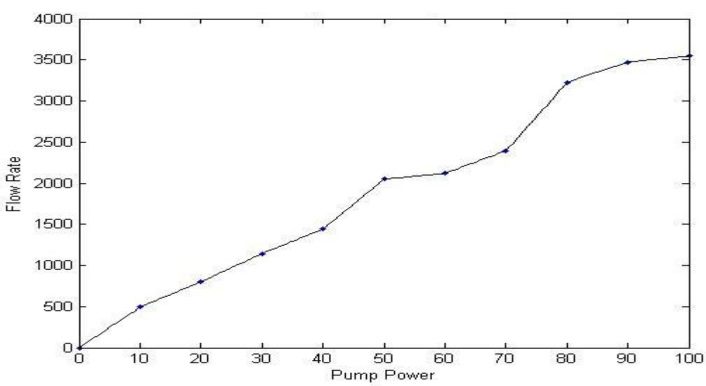

Figure 1: Linear spline

For the given data, we used quadratic spline interpolation method in MATLAB. As shown in the Figure 2, quadratic spline oscillates and overshoots too much. Because of it quadratic splines are rarely used for interpolation for practical purposes. Ideally quadratic splines are only used to understand cubic splines.

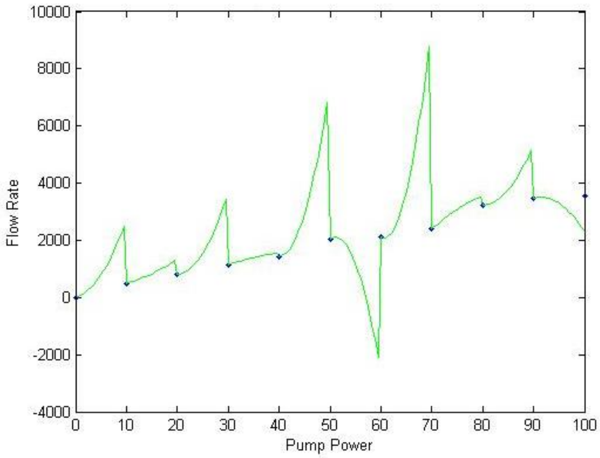

Figure 2: Quadratic spline

Now, we used natural cubic spline interpolation method in MATLAB. As shown in the Figure 3, cubic spline has two continuous derivatives, which provides visually pleasing representation of the function. But at the same time, natural cubic spline can't guarantee to preserve shape and sometimes it oscillates and overshoots. In this case, it's better to use linear spline.

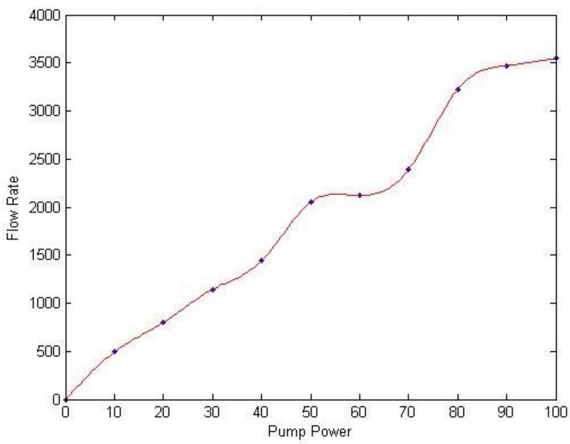

Figure 3: Cubic spline

Finally, cubic Hermite spline interpolation method was used to fit the data through MATLAB GUI. As shown on the Figure 4, cubic Hermite spline has one continuous derivative; it guarantees to preserve shape, never oscillates and over shoots. If function and derivative values are given in advance, Hermite spline is faster than cubic spline, otherwise it is twice as expensive.

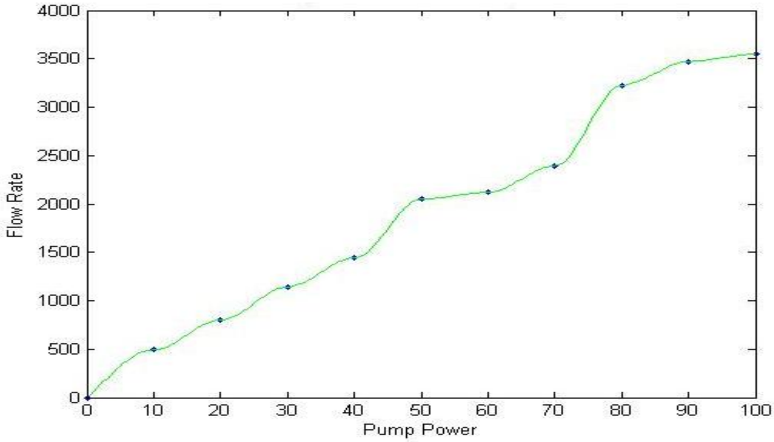

Figure 4: Cubic hermite spline

To illustrate the differences three interpolants, linear, cubic and cubic Hermite, are shown in the Figure 5, (quadratic interpolation method is not included because of too much oscillation).

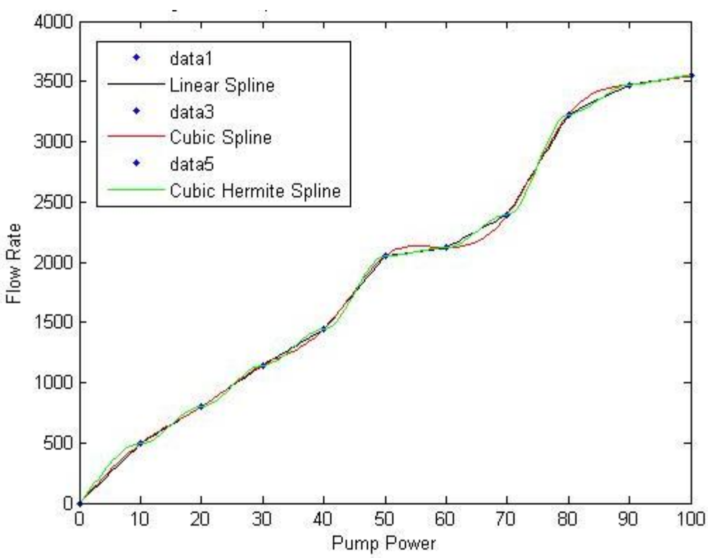

Figure 5: Comparison of Linear, cubic and cubic hermite spline

Figure 5 shows that the Cubic Hermite Interpolation has more pleasing visual appearance than linear and cubic; also it allows flexibility to preserve monotonicity.

4. Conclusion

Chemical Engineers deal with a lot of data that are crucial for modeling, process analysis, and process design. Data are often obtained or given for discrete values along a continuum, from which we often require a trend analysis or estimates at intermediate points. If we are developing a mathematical model for a certain process or physical phenomenon, we may also need to obtain some model parameters fitted to experimental data. The procedure that we need for these purposes is called curve fitting.

Based on our observations for the data we have used information from Flow Rate vs. Pump Power Table, we conclude:

1. Linear Spline is a good way of representing spray dryer results. Because it never overshoots the data and preserves monotonicity. The drawback of Linear Spline is, it is not smooth and it does not represent the real behavior of the function.
2. Quadratic Splines oscillates and overshoots the data extremely, it does not have any scientific value for our data.
3. Cubic Splines are visually pleasing. Even though they may oscillate for some data, they produce reasonable fit to the data we used.
4. For our spray dryer results, Cubic Hermite is showing the best behavior. It does not overshoot, it preserves the shape, it is smooth and monotonic.
5. As a result, for this specific Flow Rate Data, Cubic Hermite Interpolation is the best curve fitting approximation method.
6. The compact analysis of given data is also possible.

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