Splines and applications

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Contents

Splines and applications

- 1. History of splines
- 2. What is a spline?
- 3. Piecewise Polynomial and Splines
- 4. Natural Cubic Splines
- 5. Methods
 - 5.1 Function spline
- 6. Applications
 - 6.1 Maple Spline Function
 - 6.2 Interpolation with splines

Contents

Splines and applications

7. Implementation of Spline
7.1 A programme for calculating spline
7.2 Testing
8. Glossary
9. Bibliography

- originally developed for ship-building in the days before computer modeling.
- Pierre Bézier

- 2. What is a spline?
- simply a curve
- In mathematics a spline is a special function defined piecewise by polynomials. In computer science the term spline refers to a piecewise polynomial curve.
- The solution was to place metal weights (called knots) at the control points, and bend a thin metal or wooden beam (called a spline) through the weights.



http://www.macnaughtongroup.com/s pline_weights.htm

1.) <u>A piecewise polynomial ftn f(x) is obtained by dividing of X into contiguous intervals, and representing f(x) by a separate polynomial in each interval.</u>



- The polynomials are joined together at the interval endpoints (knots) in such a way that a certain degree of smoothness of the resulting function is guaranteed.

Denote by $h_j(X) : IR \to IR$ the *j*th transformation of X, j=1...M. We then model

a linear basis expansion in X.

2.) A piecewise constant:

 $f(X) \approx \sum_{j=1}^{m} \beta_j h_j(X)$



- basis function :

$$h_1(X) = 1_{X < \xi_1}$$
 $h_2(X) = 1_{\xi_1 \le X < \xi_2}$ $h_3(X) = 1_{\xi_2 \le X}$

This panel shows a piecewise constant function fit to some artificial data. The broken vertical lines indicate the position of the two knots ξ₁ and ξ₂.
The blue curve represents the true function.

3.) A piecewise linear



- basis function : three additional basis ftn are needed

$$h_{m+3} = h_m(X)X, \ m = 1, \dots, 3$$

the panel shows piecewise linear function fit to the data.
unrestricted to be continuous at the knots.

4.) continous piecewise linear



- restricted to be continuous at the two knots.
- linear constraints on the parameters:

 $f(\xi_1^-) = f(\xi_1^+)$ implies that $\beta_1 + \xi_1 \beta_4 = \beta_2 + \xi_1 \beta_5$.

- the panel shows piecewise linear function fit to the data.

- restricted to be continuous at the knots.

7.) Piecewise cubic polynomial



- - The function in the lower right panel is continuous and has continuous first and second derivatives.
- - It is known as a **cubic spline.**
- - basis function:

$h_1(X) = 1$	$h_3(X) = X^2$	$h_5(X) = (X - \xi_1)^3_+$
$h_2(X) = X$	$h_4(X) = X^3$	$h_6(X) = (X - \xi_2)^3_+$

- the pictures show a series of piecewise-cubic polynomials fit to the same data, with increasing orders of continuity at the knots.

8.) <u>An order-M spline with knot</u> $\xi_j, j = 1, \dots, K$ is a piecewise-polynomial of order M, and has continuous derivatives up to order M-2.

- a cubic spline has M=4. Cubic splines are the lowest-oder spline for which the knotdiscontinuity is not visible to the human eye.

- the piecewise-constant function is an order-1 spline, while the continuous piecewise linear function is an order-2 spline.

In practice the most widely used orders are M=1,2 and 4.

4. Natural Cubic Splines

Natural Cubic Splines

<u>Cubic spline</u> is a spline constructed of piecewise third-order polynomials which pass through a set of m control points.

The second derivate of each polynomial is commonly set to zero at the endpoints, since this provides a boundary condition that completes the system of m-2 equations.

This produces a so-called "natural" cubic spline and leads to a simple tridiagonal system which can be solved easily to give the coefficients of the polynomials.

5. Methods

5.1 Function Spline

spline(x,y,z,d);

- x,y two vectors or two lists
- z name
- d (optional) positive integer or string

The spline function computes a piecewise polynomial approximation to the X Y data values of degree d (default 3) in the variable z. The X values must be distinct and in ascending order. There are no conditions on the Y values.

6.1 Maple Spline Function: y=sin(x) and **x=[0,6]**

- > plot(sin(x),x=0..6);
- > **f:=x->sin**(**x**);
- > x1:=[0,1,2,3,4,5,6];
- > fx1:=map(f,x1);
- > plot([sin(x),spline(x1,fx1,x,'linear')],x=0..6,color=[red,blue],style=[line,line]);
- > plot([sin(x),spline(x1,fx1,x,'cubic')],x=0..6,color=[red,blue],style=[line,line]);
- > plot([sin(x),spline(x1,fx1,x,2)],x=0..6,color=[red,blue],style=[line,line]);



6.2 Interpolation with cubic spline

The function is $f(x)=\sin(\pi/2^*x)$, $x \in [-1,1]$. Interpolant the function on -1, 0, 1 with cubic spline, which satisfied the following boundary conditions:

S'(-1)=f'(-1)=0 S'(1)=f'(1)=0

One seeks the cubic spline in the following form:

$$S(x) = \begin{cases} P_1(x) = a_1 x^3 + b_1 x^2 + c_1 x + d_1, \text{ ha } x \in [-1; 0] \\ P_2(x) = a_2 x^3 + b_2 x^2 + c_2 x + d_2, \text{ ha } x \in [0; 1] \end{cases}$$

By stating the interpolant conditions, the continuity of the spline is satisfied:

1)
$$S(-1) = P_1(-1) = f(-1) \iff -a_1 + b_1 - c_1 + d_1 = -1$$

2) $S(0) = P_1(0) = f(0) \iff d_1 = 0$
3) $S(0) = P_2(0) = f(0) \iff d_2 = 0$
4) $S(1) = P_2(1) = f(1) \iff a_2 + b_2 + c_2 + d_2 = 1$

6.2 Interpolation with cubic spline

In the same time the first and the second derivate of the spline needs to be also

continous:

$$P_{i}'(x) = 3a_{i}x^{2} + 2b_{i}x + c_{i}, P_{i}'(x) = 6a_{i}x + 2b_{i}, (i = 1, 2)$$
5) $P_{1}'(0) = P_{2}'(0) \iff c_{1} = c_{2}$
6) $P_{1}''(0) = P_{2}''(0) \iff b_{1} = b_{2}$

One obtains 6 equations involving 8 unknows, and in this way the Hermite condition needs to be taken into account:

7)
$$P_1'(-1) = 3a_1 - 2b_1 + c_1 = 0$$

8) $P_2'(1) = 3a_2 + 2b_2 + c_2 = 0$

Solve the system of equations. By using the equations 2), 3), 5) and 6) one can reduce the original system:

1)
$$-a_1 + b_1 - c_1 = -1$$

4) $a_2 + b_1 + c_1 = 1$
7) $3a_1 - 2b_1 + c_1 = 0$
8) $3a_2 + 2b_1 + c_1 = 0$

6.2 Interpolation with cubic spline

Solving this:

One obtains a1-a2=0 and a1+a2=-1 => a1=a2=-1/2. Finally the sought spline reads as follows:

$$S(x) = \begin{cases} -\frac{1}{2}x^3 + \frac{3}{2}x, \text{ ha } x \in [-1; 0] \\ -\frac{1}{2}x^3 + \frac{3}{2}x, \text{ ha } x \in [0; 1] \end{cases}.$$

7.1 A programme for calculating spline

```
- procedure polynom creation
```

```
> creation_poly:=proc(d1,d2,x1,x2,y1,y2)
    local x,h:
```

```
h:=x2-x1:
unapply(y1*(x2-x)/h + y2*(x-x1)/h
-h*h/6*d1*((x2-x)/h-((x2-x)/h)^3)
-h*h/6*d2*((x-x1)/h-((x-x1)/h)^3),x)
end:
```

- Procedure spline

```
> s:=proc(x::list(numeric),y::list(numeric))
    local n,i,j,mat,res,sol,draw,h1,h2,pol:
    if nops(x)<>nops(y) then ERROR(,,number of x and y most be equal'') fi:
    n:=nops(x):
    mat:=[1,seq(0,j=1..n-1)],[seq(0,j=1..n-1),1]:
    res:=0.0:
    for i from 2 to n-1 do
    h1:=x[i]-x[i-1]:
    h2:=x[i+1]-x[i]:
    mat:=[seq(0,j=1..i-2),h1*h1,2*(h1*h1+h2*h2),h2*h2,seq(0,j=1..n-i-1)],mat:
    res:=6*(y[i+1]-2*y[i]+y[i-1]),res:
    od:
    sol:=linsolve([mat],[res]):
    draw:=NULL:
    for i to n-1 do
    pol:=creation_poly(sol[i],sol[i+1],x[i],x[i+1],y[i],y[i+1]):
    draw:=plot(pol(z),z=x[i]..x[i+1]),draw:
    od:
    eval(draw):
    end:
```

7.2 Testing the programme

> test1:=s([0,1/4,1/2,3/4,1],[0,1/16,1/4,9/16,1]):
> display(test1,plot(x^2,x=0..1,color=blue));



7.2 Testing the programme

> test2:=s([0,1/100,1/25,1/16,1/4,16/25,1],[0,1/10,1/5,1/4,1/2,4/5,1]):
> display(test2,plot(sqrt(x),x=0..1,color=blue), view=[0..1,0..1]);



8. Glossary

piecewise: a piecewise-defined function f(x) of a real variable x is a function whose definition is given differently on disjoint intervals of its domain. A common example is the absolute value function. **<-BACK**

spline: in mathematics a spline is a special function defined piecewise by polynomials. In computer science the term spline refers to a piecewise polynomial curve. **<-BACK**

cubic spline: is a spline constructed of piecewise third-order polynomials which pass through a set of m control points. The second derivate of each polynomial is commonly set to zero at the endpoints, since this provides a boundary condition that completes the system of m-2 equations. This produces a so-called "natural" cubic spline and leads to a simple tridiagonal system which can be solved easily to give the coefficients of the polynomials. **<-BACK**

9. Bibliography

Jerome Friedman, Trevor Hastie, Robert Tibshirani (2001). The Elements of Statistical Learning, Basis expansion and regularization: 115-164.

Course (2001-2002). Symbolic and Numerical Computation. "Babes-Bolyai" University

Basis expansion and regularization – from site of Seoul National University

http://stat.snu.ac.kr/prob/seminar/ElementsOfStatisnow/earning/Chapter5.ppt

Spline Cubic – from Wolfram MathWorld http://mathworld.wolfram.com/CubicSpline.html

Piecewise – Wikipedia the free encyclopedia <u>http://en.wikipedia.org/wiki/Piecewise</u>

Splines – from site of University of Oregon <u>http://www.uoregon.edu/~greg/math352-04w/splines.pdf</u>

Spline weight image – from site of MacNaughton Yacht Designs <u>http://www.macnaughtongroup.com/spline_weights.htm</u>