Natural Cubic Spline

very high order polynomials oscillate and give undesired feature

lower order splines do not oscillate, but are not very smooth at the joints (knots) where they may change their character (shape)

the derivative of the first order spline may not be continuous, the slope of the spline may change abruptly at the knots

the second derivative of the second order spline may not be continuous. the curvature of the quadratic spline may change abruptly at the knots

a better strategy is to use moderate order polynomials to construct spline and to impose smoothness conditions at the knots so that the resulting spline looks smooth but not oscillatory

Spline of Degree k

a function S is a spline of degree k if

1.) the domain of S is an interval $[a, b]$

2.) $S, S', \ldots, S^{(k-1)}$, are all continuous function on $[a, b]$

3.) there are points t_i (the knots of S) such that $a = t_0 < t_1 < \cdots < t_n = b$ and such that S is a polynomial of degree at most k on each subinterval $[t_i, t_{i+1}]$

smoothness is reflected by the order of the continuous derivative at the knots

if we want the approximating spline to have continuous mth derivative, we should choose a spline of degree at least $m + 1$

Cubic Spline

for a spline of degree $(m+1)$ at any interior knot t_i, we have

$$\lim_{x \to t_i^-} S^{(k)}(x) = \lim_{x \to t_i^+} S^{(k)}(x) \quad (0 \le k \le m)$$

since different polynomials are defined at different side of t_i, these two polynomials will be the same if they are at most degree m and their zeroth to mth derivatives are equal

in most applications, a spline of degree 3 is chosen (smooth and cheap to construct)

this spline has continuous first and second derivatives

its graph looks smooth, although higher derivatives may be discontinuous

Natural Cubic Spline

given a table of data set

x	t_0	t_1	$\cdots$	t_n
y	y_0	y_1	$\cdots$	y_n

where the t_i's are the knots in ascending order

we want to construct a function S with n piecewise cubic polynomials

$$S(x) = \begin{cases} S_0(x) & t_0 \leq x \leq t_1 \\ S_1(x) & t_1 \leq x \leq t_2 \\ \vdots & \vdots \\ S_{n-1}(x) & t_{n-1} \leq x \leq t_n \end{cases}$$

$S_i(x)$ is the cubic polynomial defined on the subinterval $[t_i, t_{i+1}]$, the cubic polynomial looks like

$$S_i(x) = a_i x^3 + b_i x^2 + c_i x + d_i \quad 0 \leq i \leq n-1$$

we have a total of $4n$ unknowns to be determined

Natural Cubic Spline

$S(x)$ must satisfy the interpolation conditions

$$S(t_i) = y_i \qquad (0 \leq i \leq n)$$

this will yield $2n$ conditions for n intervals

$S(x), S'(x)$ and $S''(x)$ have to satisfy the continuity conditions at the interior knots $t_1, t_2, \ldots, t_{n-1}$

$$\lim_{x \to t_i^-} S^{(k)}(x) = \lim_{x \to t_i^+} S^{(k)}(x) \qquad (k = 0, 1, 2)$$

this will yield $2(n-1)$ conditions

the remaining two (natural) conditions are imposed at the end knots as

$$S''(t_0) = S''(t_n) = 0$$

these particular conditions give the name of natural cubic spline. Other end knot conditions can also be imposed

Computational Algorithm

since $S''(x)$ is continuous, we define

$$z_i = S''(t_i) \qquad (0 \leq i \leq n)$$

with $z_0 = z_n = 0$. For the interval $[t_i, t_{i+1}]$ $S_i''(x)$ is continuous and takes the values of z_i and z_{i+1} at knots t_i and t_{i+1} (interpolation on interval $[t_i, t_{i+1}]$)

$$S_i''(x) = \frac{z_{i+1}}{h_i}(x - t_i) + \frac{z_i}{h_i}(t_{i+1} - x)$$

with $h_i = t_{i+1} - t_i$ for $0 \leq i \leq n-1$

it can be verified that $S_i''(t_i) = z_i, S_i''(t_{i+1}) = z_{i+1}$ for the interpolation conditions of $S_i''(x)$

if we integrate $S_i''(x)$ twice, we get $S_i(x)$

$$S_i(x) = \frac{z_{i+1}}{6h_i}(x - t_i)^3 + \frac{z_i}{6h_i}(t_{i+1} - x)^3 + cx + d$$

with c and d being two constants

Computational Algorithm (II)

the cubic polynomial can be rewritten as

$$S_i(x) = \frac{z_{i+1}}{6h_i}(x - t_i)^3 + \frac{z_i}{6h_i}(t_{i+1} - x)^3 + C_i(x - t_i) + D(t_{i+1} - x)$$

since $S_i(x)$ must also interpolate at t_i and t_{i+1} we have $S_i(t_i) = y_i$ and $S_i(t_{i+1}) = y_{i+1}$, the constants C_i and D_i can be determined

we now have the polynomial as a function of the z_i's

$$S_i(x) = \frac{z_{i+1}}{6h_i}(x - t_i)^3 + \frac{z_i}{6h_i}(t_{i+1} - x)^3 + \left(\frac{y_{i+1}}{h_i} - \frac{h_i}{6}z_{i+1}\right)(x - t_i) + \left(\frac{y_i}{h_i} - \frac{h_i}{6}z_i\right)(t_{i+1} - x)$$

Computational Algorithm (III)

in order to impose the continuity conditions for $S'(x)$, we have

$$\begin{aligned} S_i'(x) &= \frac{z_{i+1}}{2h_i}(x - t_i)^2 - \frac{z_i}{2h_i}(t_{i+1} - x)^2 \\ &\quad + \frac{y_{i+1}}{h_i} - \frac{h_i}{6}z_{i+1} - \frac{y_i}{h_i} + \frac{h_i}{6}z_i \end{aligned}$$

we have at the knot t_i

$$\begin{aligned} S_i'(t_i) &= -\frac{h_i}{6}z_{i+1} - \frac{h_i}{3}z_i + b_i \\ b_i &= \frac{1}{h_i}(y_{i+1} - y_i) \end{aligned}$$

and

$$\begin{aligned} S_{i-1}'(t_i) &= -\frac{h_{i-1}}{6}z_{i-1} - \frac{h_{i-1}}{3}z_i + b_{i-1} \\ b_{i-1} &= \frac{1}{h_{i-1}}(y_i - y_{i-1}) \end{aligned}$$

Computational Algorithm (IV)

the continuity condition implies $S'_i(t_i) = S'_{i-1}(t_i)$, i.e.,

$$h_{i-1}z_{i-1}+2(h_{i-1}+h_i)z_i+h_iz_{i+1} = 6(b_i-b_{i-1})$$

for $1 \le i \le n-1$. we then have to solve a tridiagonal system of equations

$$\begin{aligned} z_0 &= 0 \\ h_{i-1}z_{i-1} + u_iz_i + h_iz_{i+1} &= v_i \quad (1 \le i \le n-1) \\ z_n &= 0 \end{aligned}$$

with

$$\begin{aligned} u_i &= 2(h_{i-1} + h_i) \\ v_i &= 6(b_i - b_{i-1}) \end{aligned}$$

note that we have a tridiagonal system to solve

it can be shown that pivoting is not needed to solve the tridiagonal system

Smoothness of Cubic Spline

the smoothness of an interpolation polynomial can be measured in some sense by the degree of fluctuation of its derivatives

the cubic spline can be shown as "smooth"

if S is the natural cubic spline function that interpolates a twice continuously differentiable function f at knots $a = t_0 < t_1 < \cdots < t_n = b$, then

$$\int_a^b [S''(x)]^2 \, dx \leq \int_a^b [f''(x)]^2 \, dx$$

if the graph of a function changes abruptly at some knot, we can construct two different natural cubic splines at different side of that knot to avoid forcing derivative continuity at a point where the function's derivative is not continuous