Cubic spline interpolation with periodic boundary conditions.

1 Introduction

The problem of cubic spline interpolation with periodic boundary conditions can be solved with following steps:

1. Find first derivatives of interpolating function in the given points using numeric algorithms.
2. Build up cubic polynomial in Hermit form for each interval.

2 Polynomial in Hermit form

Firstly compose cubic polynomial on a single interval $[a,\, b]$:
Denote:

$$h = \frac{1}{x_b - x_a}$$

Consequence of Lagrange's formula:

$$p_1(x) = y_b \cdot (x - x_a)\; h + y_a \cdot (x_b - x)\; h$$
$$p_1(x_a) = y_a$$
$$p_1(x_b) = y_b$$

Let's make up cubic polynomial p_3 so that

$$p_3(x) = p_1(x) + \dots$$
$$p_3(x_a) = y_a,\, p_3(x_b) = y_b$$
$$p_3'(x_a) = s_a,\, p_3'(x_b) = s_b$$

Suppose that values of s_a and s_b are known.

$$p_3(x) = y_b(x - x_a)\; h + y_a(x_b - x)\; h + (x - x_a)\; h \cdot (x_b - x)\; h\, [A(x - x_a) + B(x_b - x)]$$

Finding A and B:

$$p_3'(x) = (y_b - y_a) \cdot h + (x_b - x) \cdot h^2\, [A(x - x_a) + B(x_b - x)] -$$
$$-(x - x_a) \cdot h^2\, [A(x - x_a) + B(x_b - x)] + (x - x_a)(x_b - x) \cdot h^2\, [A - B]$$

Denote by

$$m = \frac{y_b - y_a}{x_b - x_a}$$

Include x_a and x_b in $p_3'(x)$:

$$\begin{gathered} p_3'(x_a) = m + B = s_a \Rightarrow B = s_a - m \\ p_3'(x_b) = m - A = s_b \Rightarrow A = m - s_b \end{gathered}$$

We got cubic polynomial in Hermit form for the single interval:

$$p_3(x) = y_b(x - x_a)\ h + y_a(x_b - x)\ h + (x - x_a)\ h \cdot (x_b - x)\ h\,[(m - s_b)(x - x_a) + (s_a - m)(x_b - x)] \tag{1}$$

3 First derivatives

To find the dependence between the polynomials in Hermit form in the neighboring intervals we need to find the second derivatives of these polynomials (because interpolation is made with splines) $p_3''(x)$:

$$p_3''(x) = -2h^2(s_b - m)\,[(x_b - x) - 2(x - x_a)] - 2h^2(s_a - m)\,[2(x_b - x) - (x - x_a)]$$

Find the value of polynomial $p_3''(x)$ in boundary points x_a and x_b:

$$\begin{gathered} p_3''(x_a) = -2h(s_b - m) - 4h(s_a - m) \\ p_3''(x_b) = 4h(s_b - m) + 4h(s_a - m) \end{gathered}$$

Build up polynomials $p_{3,k}$, $k = 0, \ldots, n$ on each of the intervals $[x_{k-1},\ x_k]$ which will form a spline interpolating function.

$$\begin{gathered} x_a = x_k,\ x_b = x_{k+1}, \\ s_a = s_k,\ s_b = s_{k+1}, \\ h = h_k = \frac{1}{x_{k+1} - x_k} \\ m = m_k = \frac{y_{k+1} - y_k}{x_{k+1} - x_k} \end{gathered}$$

$$\begin{gathered} p_{3,k}(x) = y_{k+1}(x - x_k)\ h_k + y_k(x_{k+1} - x)\ h_k + \\ +(x - x_k)\ h_k \cdot (x_{k+1} - x)\ h_k\,[(m_k - s_k)(x - x_k) + (s_{k-1} - m_k)(x_{k+1} - x)] \\ p_{3,k}''(x_k) = -2h_k(s_{k+1} - m_k) - 4h_k(s_k - m_k) \\ p_{3,k}''(x_{k+1}) = 4h_k(s_{k+1} - m_k) + 4h_k(s_k - m_k) \end{gathered}$$

Constraint of cubic spline:

$$p_{3,k-1}''(x_k) = p_{3,k}''(x_k)$$

We can replace it with the second derivative of a polynomial in Hermite form:

$$(2h_{k-1}s_{k-1} + 4h_{k-1}s_k) - 6h_{k-1}m_{k-1} = -(4h_k s_k + 2h_k s_{k+1}) + 6h_k m_k$$

With regrouping equation above, we get a linear system of equations:

$$h_{k-1}s_{k-1} + 2(h_{k-1} + h_k)s_k + h_k s_{k+1} = 3h_{k-1}m_{k-1} + 3h_k m_k$$

This system can be rewritten in matrix form with almost tridiagonal matrix (here we use **cyclic boundary condition**: $s_{-1} = s_n,\ s_0 = s_{n+1}$):

$$A = \begin{pmatrix} 2h_n + 2h_0 & h_0 & 0 & 0 & & 0 & h_n \\ h_0 & 2h_0 + 2h_1 & h_2 & 0 & & 0 & 0 \\ & \ddots & \ddots & \ddots & & & \\ & & & & & & \\ & & & \ddots & \ddots & \ddots & 0 \\ 0 & & & 0 & h_{n-2} & 2h_{n-2} + 2h_{n-1} & h_{n-1} \\ h_n & 0 & & 0 & 0 & h_{n-1} & 2h_{n-1} + 2h_n \end{pmatrix}$$

$$x = \begin{pmatrix} s_0 \\ s_1 \\ \vdots \\ s_n \end{pmatrix},\ b = \begin{pmatrix} h_n m_n + h_0 m_0 \\ h_0 m_0 + h_1 m_1 \\ \vdots \\ h_{n-1} m_{n-1} + h_n m_n \end{pmatrix}$$

Matrix A is almost tridiagonal, but it can be broken down into the sum of a tridiagonal matrix and a correction, $A = B + uv^T$, where

$$u = \begin{pmatrix} h_n \\ 0 \\ \vdots \\ 0 \\ h_n \end{pmatrix},\ v = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$$

and then find values of the first derivatives in the given points using the Sherman–Morrison formula: for system

$$(B + uv^T)x = b$$

we have to solve two auxiliary systems:

$$By = b,\ Bz = u$$

This systems can be solved using the Thomas algorithm (because in both systems B is the tridiagonal matrix).
After this, vector x will be found using a formula:

$$x = y - \left[\frac{vy}{1 + vz}\right] z$$