Differential Approach in Spline Theory

Boris Kvasov*

Institute of Computational Technologies, Russian Academy of Sciences
Lavrentyev Avenue 6, Novosibirsk, 630090 Russia
email: kvasov@ict.nsc.ru

A method for constructing interpolation splines by solving differential multipoint boundary value problems (DMBVP) with subsequent discretization was described in [2, 3]. In comparison with the standard algebraic approach [5, 7], this method does not involve hyperbolic/biharmonic function evaluation, but requires the solution of a five-diagonal system, which can be ill-conditioned for unequally spaced data (see [4]). It is shown below that this system can be split into a set of positive five-diagonal linear ones and admit effective parallelization.

1 1-D Problem Formulation

Suppose that we are given the data

$$(x_i, f_i), \quad i = 0, \ldots, N+1, \tag{1}$$

where $a = x_0 < x_1 < \ldots < x_{N+1} = b$. Define

$$f[x_i, x_{i+1}] = (f_{i+1} - f_i)/h_i, \quad h_i = x_{i+1} - x_i, \quad i = 0, \ldots, N.$$

Data (1) are called monotonically increasing if

$$f[x_i, x_{i+1}] \geq 0, \quad i = 0, \ldots, N,$$

and are called convex if

$$f[x_i, x_{i+1}] \geq f[x_{i-1}, x_i], \quad i = 1, \ldots, N.$$

The shape preserving interpolation problem consists in constructing a sufficiently smooth function S such that $S(x_i) = f_i$ for $i = 0, \ldots, N+1$ and S is monotone/convex on the intervals of monotonicity/convexity of the input data.

Obviously, the solution to the shape preserving interpolation problem is not unique. We seek it in the form of a hyperbolic tension spline.

Definition 1. *The hyperbolic interpolation spline S with the set of tension parameters $\{p_i \geq 0 \mid i = 0, \ldots, N\}$ is defined as the solution to the DMBVP*

$$\frac{d^4\mathrm{S}}{dx^4} - \left(\frac{p_i}{h_i}\right)^2 \frac{d^2\mathrm{S}}{dx^2} = 0 \quad \text{for all} \quad x \in (x_i, x_{i+1}), \quad i = 0, \ldots, N, \tag{2}$$

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$$\mathrm{S} \in C^2[a,b] \tag{3}$$

with the interpolation conditions

$$\mathrm{S}(x_i) = f_i, \quad i = 0, \dots, N+1 \tag{4}$$

and the boundary conditions

$$\mathrm{S}''(a) = f_0'' \quad \text{and} \quad \mathrm{S}''(b) = f_{N+1}''. \tag{5}$$

Boundary conditions (5) are used for simplicity. They can be replaced by boundary conditions of other types [3].

The second derivative values in the endpoint conditions (5) must be adjusted to the behaviour of the data. Otherwise we can obtain an incompatibility with the shape preserving restrictions [3]. For example, we can use the restrictions

$$f_0'' f[x_0, x_1, x_2] \geq 0, \quad f_{N+1}'' f[x_{N-1}, x_N, x_{N+1}] \geq 0.$$

If we set $p_i = 0$ for all i in (2), then the solution to problem (2)–(5) is a cubic spline of the class C^2, which gives a smooth curve but does not always preserve the monotonicity/convexity of the input data. In the limit as $p_i \to \infty$, we obtain a polygonal line that is shape preserving for the input data but is not smooth. In standard algorithms for automatic selection of the shape parameters p_i (see [3]), the latter are chosen so that the resulting curve is as much similar to a cubic spline as possible and simultaneously preserves the monotonicity/convexity of the input data.

2 Finite Difference Approximation

Consider the discretization of the DMBVP formulated. For this purpose, on each subinterval $[x_i, x_{i+1}]$, we introduce an additional nonuniform mesh

$$x_{i,-1} < x_i = x_{i,0} < x_{i,1} < \cdots < x_{i,n_i} = x_{i+1} < x_{i,n_i+1}, \quad n_i \in \mathbb{N}$$

with the steps $h_{ij} = x_{i,j+1} - x_{ij}$, $j = -1, \dots, n_i$, $i = 0, \dots, N$. We search for a mesh function

$$\{ \ u_{ij}, \ j = -1, \dots, n_i + 1, \ i = 0, \dots, N \ \},$$

satisfying the difference equations

$$\begin{aligned} 24u[x_{i,j-2}, \dots, x_{i,j+2}] - 2\Big(\frac{p_i}{h_i}\Big)^2 u[x_{i,j-1}, x_{ij}, x_{i,j+1}] \ = \ 0, \\ j = 1, \dots, n_i - 1, \quad i = 0, \dots, N. \end{aligned} \tag{6}$$

The approximation of smoothness conditions (3) gives the relations

$$\begin{aligned} u_{i-1,n_{i-1}} &= u_{i,0}, \\ D^1_{i-1,n_{i-1}} u_{i-1,n_{i-1}} &= D^1_{i,0} u_{i,0}, \quad i = 1, \dots, N, \\ D^2_{i-1,n_{i-1}} u_{i-1,n_{i-1}} &= D^2_{i,0} u_{i,0}, \end{aligned} \tag{7}$$

where

$$D^1_{ij}u_{ij} = \lambda_{ij}u[x_{i,j-1}, x_{ij}] + (1-\lambda_{ij})u[x_{ij}, x_{i,j+1}],$$
$$D^2_{ij}u_{ij} = 2u[x_{i,j-1}, x_{ij}, x_{i,j+1}], \quad \lambda_{ij} = h_{ij}/(h_{i,j-1}+h_{ij}).$$

Conditions (4) and (5) are transformed into

$$u_{i,0} = f_i, \quad i = 0, \dots, N, \quad u_{N,n_N} = f_{N+1} \tag{8}$$

and

$$u[x_{0,-1}, x_{0,0}, x_{0,1}] = f''_0, \quad u[x_{N,n_N-1}, x_{N,n_N}, x_{N,n_N+1}] = f''_{N+1}. \tag{9}$$

Relations (7) and boundary conditions (9) make it possible to eliminate the "extra" unknowns $u_{i,-1}$ and u_{i,n_i+1}, $i = 0, \dots, N$. To show this we use the notation

$$M_i = 2u[x_{i-1,n_{i-1}-1}, x_{i-1,n_{i-1}}, x_{i-1,n_{i-1}+1}] = 2u[x_{i,-1}, x_{i,0}, x_{i,1}].$$

Multiplying these equalities by $h_{i-1,n_{i-1}-1}/2$ and $h_{i,0}/2$, respectively, we rewrite them in the form

$$D^1_{i-1,n_{i-1}}u_{i-1,n_{i-1}} = u[x_{i-1,n_{i-1}-1}, x_{i-1,n_{i-1}}] + \frac{h_{i-1,n_{i-1}-1}}{2}M_i,$$
$$D^1_{i,0}u_{i,0} = u[x_{i,0}, x_{i,1}] - \frac{h_{i,0}}{2}M_i.$$

Using the second equality in (7) we obtain

$$M_i = 2u[x_{i-1,n_{i-1}-1}, x_{i,0}, x_{i,1}], \quad i = 1, \dots, N. \tag{10}$$

Thus the second divided differences in the equations (6) of the form

$$u[x_{i-1,n_{i-1}-1}, x_{i-1,n_{i-1}}x_{i-1,n_{i-1}+1}] \quad \text{and} \quad u[x_{i,-1}, x_{i,0}, x_{i,1}]$$

can be replaced by $u[x_{i-1,n_{i-1}-1}, x_{i,0}, x_{i,1}]$. This permits us to eliminate the unknowns $u_{i-1,n_{i-1}+1}$ and $u_{i,-1}$, $i = 1, \dots, N$. The unknowns $u_{0,-1}$ and u_{N,n_N+1} are eliminated from boundary conditions (9). The discrete *mesh solution* is defined as

$$\{\ u_{ij},\ j = 0, \dots, n_i,\ i = 0, \dots, N\ \}. \tag{11}$$

The existence and uniqueness conditions of a solution to linear system (6)–(9) will be obtained below.

3 Parallel Algorithm for Five-Diagonal System

Let us consider the quasiuniform mesh which is uniform separately on each interval $[x_i, x_{i+1}]$, $i = 0, \dots, N$, i.e. $h_{ij} = \tau_i$ for $j = -1, \dots, n_i$. In this case the system (6)–(9) after eliminating the unknowns $u_{i,-1}$, u_{i,n_i+1}, $i=0,\ldots,N$ takes the form

$$\mathbf{Au} = \mathbf{b}, \tag{12}$$

where

$$\mathbf{u} = (u_{0,1},\ldots,u_{0,n_0-1},u_{1,1},\ldots,u_{2,1},\ldots,u_{N,1},\ldots,u_{N,n_N-1})^T,$$

$$\begin{aligned}\mathbf{b} = (&-(a_0+2)f_0-\tau_0^2 f_0'', -f_0,\ 0,\ldots,0,-f_1,-\gamma_{0,n_0-1}f_1,-\gamma_{1,1}f_1,\\ &,-f_1,0,\ldots,\ 0,-f_{N+1},-(a_N+2)f_{N+1}-\tau_N^2 f_{N+1}'')^T\end{aligned}$$

with

$$\gamma_{i-1,n_{i-1}-1} = a_{i-1}+2\frac{\rho_i-1}{\rho_i},\quad \gamma_{i,1}=a_i+2(1-\rho_i),\quad i=1,\ldots,N$$

and $\mathbf{A}$ is the following five-diagonal matrix

$$\begin{bmatrix}
b_0-1 & a_0 & 1 & & & & & & & & & & \\
a_0 & b_0 & a_0 & 1 & & & & & & & & & \\
1 & a_0 & b_0 & a_0 & 1 & & & & & & & & \\
& & & \cdots & & & & & & & & & \\
& & 1 & a_0 & b_0 & a_0 & & & & & & & \\
& & & 1 & a_0 & \eta_{0,n_0-1} & \delta_{0,n_0-1} & & & & & & \\
& & & & & \delta_{1,1} & \eta_{1,1} & a_1 & 1 & & & & \\
& & & & & & a_1 & b_1 & a_1 & 1 & & & \\
& & & & & & & & \cdots & & & & \\
& & & & & & & 1 & a_N & b_N & a_N & 1 & \\
& & & & & & & & 1 & a_N & b_N & a_N & \\
& & & & & & & & & 1 & a_N & b_N-1 &
\end{bmatrix}$$

with

$$\begin{aligned}
&a_i = -(4+\omega_i)\ ,\ b_i = 6+2\omega_i\ ,\ \omega_i = \left(\frac{p_i}{n_i}\right)^2;\quad i=0,\ldots,N,\\
&\eta_{i-1,n_{i-1}-1} = b_{i-1}+\frac{1-\rho_i}{1+\rho_i}\ ,\ \eta_{i,1}=b_i+\frac{\rho_i-1}{\rho_i+1},\quad \rho_i=\frac{\tau_i}{\tau_{i-1}},\\
&\delta_{i-1,n_{i-1}-1} = \frac{2}{\rho_i(\rho_i+1)}\ ,\ \delta_{i,1} = 2\frac{\rho_i^2}{\rho_i+1}\ ,\quad i=1,\ldots,N.
\end{aligned}$$

In [3] the system (12) is solved using five-diagonal Gaussian elimination. In the general case for unequally spaced data this system may be ill-conditioned [4]. To avoid this problem let us consider a parallel algorithm of Gaussian elimination for the solution of the system (12) based on approach [6].

We cancel equations of the system (12) which are most close to the data points x_i or more precisely the equations

$$(b_0-1)u_{0,1}+a_0u_{0,2}+u_{0,3} = -(a_0+2)f_0-\tau_0^2 f_0'',$$

$$
\begin{aligned}
&u_{i-1,n_{i-1}-3}+a_{i-1}u_{i-1,n_{i-1}-2}+\eta_{i-1,n_{i-1}-1}u_{i-1,n_{i-1}-1}\\
&\qquad\qquad\qquad +\delta_{i-1,n_{i-1}-1}u_{i,1}=-\gamma_{i-1,n_{i-1}-1}f_i, \qquad (13)\\
&\delta_{i,1}u_{i-1,n_{i-1}-1}+\eta_{i,1}u_{i,1}+a_iu_{i,2}+u_{i,3}=-\gamma_{i,1}f_i, \quad i=1,\dots,N,\\
&u_{N,n_N-3}+a_Nu_{N,n_N-2}+(b_N-1)u_{N,n_N-1}=-(a_N+2)f_{N+1}-\tau_N^2f''_{N+1}.
\end{aligned}
$$

Let numbers $u_{i,1}^{(0)}$, $u_{i,n_i-1}^{(0)}$, $i=0,\dots,N$, be given which correspond to the removed equations. The system (12) is split in $N+1$ subsystems

$$
\begin{aligned}
&u_{i,0}=f_i, \quad u_{i,1}=u_{i,1}^{(0)},\\
&u_{i,j-2}+a_iu_{i,j-1}+b_iu_{ij}+a_iu_{i,j+1}+u_{i,j+2}=0, \quad j=2,\dots,n_i-2, \qquad (14)\\
&u_{i,n_i-1}=u_{i,n_i-1}^{(0)}, \quad u_{i,n_i}=f_{i+1}\ .
\end{aligned}
$$

Let us show that the obtained systems have a unique solution which can be found by usual five-diagonal Gaussian elimination.

We rewrite the system (14) as

$$\mathbf{A}_i\mathbf{u}_i=\mathbf{f}_i,$$

where

$$
\begin{aligned}
&\mathbf{u}_i=(u_{i,2},u_{i,3},\dots,u_{i,n_i-2})^T,\\
&\mathbf{f}_i=(-a_iu_{i,1}^{(0)}-f_i,-u_{i,1}^{(0)},0,\dots,0,-u_{i,n_i-1}^{(0)},-a_iu_{i,n_i-1}^{(0)}-f_{i+1})^T.
\end{aligned}
$$

The matrix $\mathbf{A}_i$ is symmetric. We observe that

$$\mathbf{A}_i=\mathbf{C}_i+\mathbf{D}_i, \quad \mathbf{C}_i=\mathbf{B}_i^2-\omega_i\mathbf{B}_i,$$

where

$$
\mathbf{B}_i=\begin{pmatrix}-2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1\\ & & & 1 & -2\end{pmatrix}, \quad \mathbf{D}_i=\begin{pmatrix}1 & & & & \\ & 0 & & & \\ & & \ddots & & \\ & & & 0 & \\ & & & & 1\end{pmatrix}.
$$

Since,

$$\lambda_j(\mathbf{B}_i)=-2\Big(1-\cos\frac{j\pi}{m_i}\Big), \quad j=1,\dots,m_i-1, \quad m_i=n_i-2,$$

we have

$$\lambda_j(\mathbf{C}_i)=4\Big(1-\cos\frac{j\pi}{m_i}\Big)^2+2\omega_i\Big(1-\cos\frac{j\pi}{m_i}\Big), \quad j=1,\dots,m_i-1.$$

In addition, the eigenvalues of $\mathbf{D}_i$ are 0 and 1, thus we deduce from a corollary of the Courant-Fisher theorem [1] that the eigenvalues of $\mathbf{A}_i$ satisfy the following inequalities

$$\lambda_j(\mathbf{A}_i)\ge\lambda_j(\mathbf{C}_i)\ge 4\Big(1-\cos\frac{\pi}{m_i}\Big)^2+2\omega_i\Big(1-\cos\frac{\pi}{m_i}\Big).$$

Hence, $\mathbf{A}_i$ is a positive matrix and we directly obtain that the five-diagonal linear system has a unique solution which can be stably found by usual five-diagonal Gaussian elimination [1].

We obtain a solution $u_{ij}^{(0)}$, $j = 0, \ldots, n_i$, $i = 0, \ldots, N$.

Using equations (13) let us recalculate the scalars $u_{i,1}^{(0)}$, $u_{i,n_i-1}^{(0)}$, $i = 0, \ldots, N$. For $i = 1, \ldots, N$ we find

$$\begin{aligned} u_{i-1,n_{i-1}-1}^{(1)} &= \frac{1}{\Delta_i}\big(\eta_{i,1}F_{i,1}^{(0)} - \delta_{i-1,n_{i-1}-1}F_{i,2}^{(0)}\big), \\ u_{i,1}^{(1)} &= \frac{1}{\Delta_i}\big(- \delta_{i,1}F_{i,1}^{(0)} + \eta_{i-1,n_{i-1}-1}F_{i,2}^{(0)}\big), \end{aligned}$$

where

$$\begin{aligned} F_{i,1}^{(0)} &= -\gamma_{i-1,n_{i-1}-1}f_i - a_{i-1}u_{i-1,n_{i-1}-2}^{(0)} - u_{i-1,n_{i-1}-3}^{(0)}, \\ F_{i,2}^{(0)} &= -\gamma_{i,1}f_i - a_i u_{i,2}^{(0)} - u_{i,3}^{(0)}, \\ \Delta_i &= b_{i-1}b_i + (b_i - b_{i-1})\frac{1-\rho_i}{1+\rho_i} - 1. \end{aligned}$$

From first and last equations of the system (13) we calculate

$$\begin{aligned} u_{0,1}^{(1)} &= \frac{1}{1-b_0}\big((a_0+2)f_0 + \tau_0^2 f_0'' + a_0 u_{0,2}^{(0)} + u_{0,3}^{(0)}\big), \\ u_{N,n_N-1}^{(1)} &= \frac{1}{1-b_N}\big((a_N+2)f_{N+1} + \tau_N^2 f_{N+1}'' + a_N u_{N,n_N-2}^{(0)} + u_{N,n_N-3}^{(0)}\big). \end{aligned}$$

Solving repeatedly the system (14) we obtain a solution $u_{ij}^{(1)}$, $j = 0, \ldots, n_i$, $i = 0, \ldots, N$, etc. The calculations show that this algorithm is convergent.

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