Periodic Quadratic Spline

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Derive the formula for 1D Quadratic Spline with periodic boundary conditions

I. THE SPLINE PROBLEM

Suppose we have an unknown function $f(x) \in C^\infty$ defined on a domain $[a, b]$ satisfying the periodic condition, i.e.

$$\begin{aligned} f(a) &= f(b), \\ f^{[k]}(a) &= f^{[k]}(b) \quad (k \in \mathcal{N}), \end{aligned} \tag{1}$$

where $f^{[k]}(x)$ is the k-th order derivative respect to x.
And we have N samples of this function on $[a, b]$, evenly spaced. That is, we have known the values of $f(x)$ at N points, $f(x_i)$ $(i = 1, \ldots, N)$, and $x_{i+1} - x_i = \Delta$, $x_1 = a, x_N = b$.

The C^1 spline problem can be stated as:

Find a set of polynomials, $P_i(x)(i = 1, \ldots, N-1)$ defined on sections $\{[x_i, x_{i+1}]\}$, such that within each section,

$$P_i(x_i) = f(x_i), \tag{2}$$

$$P_i(x_{i+1}) = f(x_{i+1}), \tag{3}$$

and the first derivatives are continuous on the connecting points,

$$P_i'(x_{i+1}) = P_{i+1}'(x_{i+1}), \quad (i = 1, \ldots, N-2) \tag{4}$$

with the periodic boundary condition

$$P_{N-1}'(x_N) = P_1'(x_1). \tag{5}$$

Note that the periodicity in the function values has already been enforced in Eq. 2 and 3 by having $f(x_N) = f(x_1)$ as input.

It can be easily seen that Eq 2, 3, 4, and 5 pose a total $3N - 3$ constraints on the set of $N - 1$ polynomials $P_i(x)$. So, they uniquely determine a set of $N - 1$ quadratic polynomials in the form

$$P_i(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2. \tag{6}$$

For a given set of values $\{f(x_i)\}, i = 1, \ldots, N$, we can calculate the set of coefficients $\{(a_i, b_i, c_i)\}, i = 1, \ldots, N-1$ based on the above stated constraints. This is our periodic quadratic spline problem.

II. GENERAL SOLUTION

Eq. 2, 3, 4, and 5 can be generally expressed as a set of linear equations for the coefficients $\{(a_i, b_i, c_i)\}$. In fact, the equations obtained from Eq 2 is simply

$$a_i = f_i. \tag{7}$$

We've use the notation $f_i \equiv f(x_i)$. Then, Eq 3 becomes

$$b_i\Delta + c_i\Delta^2 = (f_{i+1} - f_i), i \in \{1, \ldots, N-1\}, \tag{8}$$

where $\Delta \equiv x_{i+1} - x_i$ is the step size in x.

Eq 4 can also be written out as

$$b_i + 2c_i\Delta = b_{i+1}, i \in \{1, \ldots, N-2\}, \tag{9}$$

and the boundary condition Eq 5 as

$$b_{N-1} + 2c_{N-1}\Delta = b_1. \tag{10}$$

We can first express c_i in terms of b_i's using Eq 9 and 10, that is

$$\begin{aligned} c_i &= \frac{b_{i+1} - b_i}{2\Delta}, i \in \{1, \dots, N-2\}, \\ c_{N-1} &= \frac{b_1 - b_{N-1}}{2\Delta}. \end{aligned} \tag{11}$$

Substitute Eq 11 into Eq 8, we finally have the equations for b_i,

$$\begin{aligned} b_i + b_{i+1} &= \frac{2(f_{i+1} - f_i)}{\Delta}, i \in \{1, \dots, N-2\} \\ b_{N-1} + b_1 &= \frac{2(f_N - f_{N-1})}{\Delta}. \end{aligned} \tag{12}$$

Define

$$y_i \equiv 2(f_{i+1} - f_i)/\Delta, i \in \{1, \dots, N-1\}, \tag{13}$$

we can write Eq 12 in vector form

$$\overleftrightarrow{A} \cdot \vec{b} = \vec{y}, \tag{14}$$

where

$$\overleftrightarrow{A} = \begin{pmatrix} 1 & 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 1 & 0 & \dots & 0 \\ \vdots & & & \ddots & & \vdots \\ 0 & \dots & 0 & 0 & 1 & 1 \\ 1 & 0 & \dots & 0 & 0 & 1 \end{pmatrix}, \tag{15}$$

is a $(N-1) \times (N-1)$ matrix.

In general, we can invert matrix $\overleftrightarrow{A}$ and write

$$\vec{b} = \overleftrightarrow{A}^{-1} \cdot \vec{y}, \tag{16}$$

given that $\overleftrightarrow{A}$ is invertible, i.e. $\det(\overleftrightarrow{A}) \neq 0$. However, in this particular case, $\overleftrightarrow{A}$ can be non-invertible when N is odd, $N = 2n+1$. One can check this by seeing that the vector $\vec{v} = (1, -1, 1, -1, \dots, 1, -1)^T$ is an eigenvector of $\overleftrightarrow{A}$ with 0 eigenvalue.

So, here, we'll discuss the solution to Eq 14 using a technique that is tailored to the specific form of $\overleftrightarrow{A}$, Eq 15.

To start, we sum over all the equations, and obtain

$$2 \sum_{i=1}^{N-1} b_i = \sum_{i=1}^{N-1} y_i. \tag{17}$$

Using the definition of y_i, Eq 13, and the periodicity condition on f, we can easily show that $\sum_{i=1}^{N-1} y_i = 0$. So we have

$$\sum_{i=1}^{N-1} b_i = 0. \tag{18}$$

Now, we need to differentiate the two cases, when N is odd or even.

A. N=2n+1

As discussed above, when $N = 2n+1$ is odd, we can not invert $\overleftrightarrow{A}$ to find the solution. In fact, in this case, the solubility condition places an additional requirement on $\vec{y}$.

In this case, $\overleftrightarrow{A}$ is a $2n \times 2n$ matrix. Sum over all the odd numbered equations gives us

$$\sum_{i=1}^{2n} b_i = \sum_{k=1}^{n} y_{2k-1}. \tag{19}$$

Using Eq 18, we have the condition

$$\sum_{k=1}^{n} y_{2k-1} = 0. \tag{20}$$

This is equivalent to the condition on f_i,

$$\sum_{k=1}^{n} f_{2k-1} = \sum_{k=1}^{n} f_{2k}, \tag{21}$$

which means the sum of function values on all odd indices must equal to the sum of those on the even indices, in order to have a solution for b_i's. When this condition is met, there is one degree of freedom to pick, for example, b_1. A good choice of b_1 can be $f'(x_1)$ estimated using f_1, f_2 and f_3 (See Appendix A for more details).

However, for some arbitrarily given $\{f_i\}$, Eq 21 may not be satisfied. In this case, there won't be a self-consistent solution for b_i, which means if we start with $b_1 = f'(x_1)$, and solve for all the other coefficients, using all but the last equations in Eq 12, and Eq 11, we won't be able to guarantee $P_{N-1}(x_N) = f(N)$. In general, we will either have a discontinuity in the value, or in the first derivative of f at one node, depending on which equation we have abandoned.

One technique that may be useful is to smoothly rescale the values at either the even nodes or the odd nodes, so that the solubility condition, Eq 21 is satisfied.

B. N=2n

When N is even, the linear equations for b_i are independent, an unique solution can be obtained.

We still sum over the odd numbered equations, but now, since the total number of equations is $2n-1$, the last equation is included, and instead of having the summation of b_i, we have an extra b_1. We have

$$b_1 = \sum_{k=1}^{n} y_{2k-1}. \tag{22}$$

Write it in terms of f_i, we have

$$b_1 = \frac{2}{\Delta}\left(\sum_{k=1}^{n-1} f_{2k} - \sum_{k=1}^{n-1} f_{2k+1}\right), \tag{23}$$

Starting from b_1, we can obtain b_i one by one using Eq 12.

One interesting question is how big the difference can be between the b_1 we calculated this way and the b_1 we estimated using f_1, f_2 and f_3. Appendix B is dedicated to answer this question.

Appendix A: Estimation of $f'(x_1)$ using f_1, f_2, and f_3

Since we have assumed infinite smoothness of $f(x)$, we can Taylor expand $f(x)$ near x_1, and get:

$$f(x) = f_1 + f'(x_1)(x - x_1) + \frac{1}{2} f''(x_1)(x - x_1)^2 + o\left((x - x_1)^3\right). \tag{A1}$$

Evaluate it at x_2, and x_3, we have

$$\begin{aligned} f_2 &= f_1 + f'(x_1)\Delta + \frac{1}{2} f''(x_1)\Delta^2 + o(\Delta^3), \\ f_3 &= f_1 + 2f'(x_1)\Delta + 2f''(x_1)\Delta^2 + o(\Delta^3), \end{aligned} \tag{A2}$$

where we have used $x_2 = x_1 + \Delta$, and $x_3 = x_1 + 2\Delta$.

In order to get $f'(x_1)$ with second order accuracy in Δ, we need to cancel the $f''(x_1)$ terms. This can be easily done by taking $4f_2 - f_3$, i.e.

$$4f_2 - f_3 = 3f_1 + 2f'(x_1)\Delta + o(\Delta^3). \tag{A3}$$

So, we have

$$f'(x_1) = \frac{4f_2 - f_3 - 3f_1}{2\Delta} + o(\Delta^2). \tag{A4}$$

Appendix B: Difference between b_1 calculated and b_1 estimated

In this part, we take $f(x) = \exp(\mathrm{j}2\pi Mx)$ on $[0, 1]$, where M is an integer, $\mathrm{j} \equiv \sqrt{-1}$ is the unit of imaginary number. It is clear that $f(x)$ is a periodic function on $[0, 1]$ with infinitely smooth derivatives.

Taking $N = 2n$ samples on $[0, 1]$ including the two end points, is actually cutting the range into $2n-1$ sections, i.e.

$$x_i = (i-1)\Delta, i \in \{1, 2, \ldots, 2n\}, \tag{B1}$$

with $\Delta = 1/(2n-1)$.

So, the $\{f_i\}$ values are

$$f_i = \exp\left(\frac{\mathrm{j}2M(i-1)\pi}{2n-1}\right). \tag{B2}$$

Substitute into our solution for b_1, Eq 23, we have

$$b_1 = (4n-2)\sum_{k=1}^{n-1}\left[\exp\left(\frac{\mathrm{j}2(2k-1)M\pi}{2n-1}\right) - \exp\left(\frac{\mathrm{j}4kM\pi}{2n-1}\right)\right]. \tag{B3}$$

Noting that $\exp(j2M\pi) = 1$, we have

$$\sum_{k=1}^{n-1}\exp\left(\frac{\mathrm{j}2(2k-1)M\pi}{2n-1}\right) = -\frac{1}{1+\exp(\mathrm{j}2M\pi/(2n-1))}, \tag{B4}$$

$$\sum_{k=1}^{n-1}\exp\left(\frac{\mathrm{j}4kM\pi}{n}\right) = -\frac{\exp(\mathrm{j}2M\pi/(2n-1))}{1+\exp(\mathrm{j}2M\pi/(2n-1))}. \tag{B5}$$

So, finally, we have

$$b_1 = (4n-2)\frac{-1+\mathrm{e}^{\mathrm{j}2M\pi/(2n-1)}}{1+\mathrm{e}^{\mathrm{j}2M\pi/(2n-1)}} = \mathrm{j}(4n-2)\tan\left(M\pi/(2n-1)\right). \tag{B6}$$

When $\delta \equiv M\pi/(2n-1) \ll 1$, we can expand the tan function, and obtain the approximated form

$$b_1 = \mathrm{j}2\pi M\left(1 + \frac{\delta^2}{3} + o(\delta^4)\right). \tag{B7}$$

The b_1 calculated using the estimation formula Eq A4 will be

$$b_1^e = (2n-1)(4\mathrm{e}^{\mathrm{j}2\delta} - \mathrm{e}^{\mathrm{j}4\delta} - 3)/2 = \mathrm{j}2\pi M\left(1 + \frac{4\delta^2}{3} + o(\delta^3)\right). \tag{B8}$$

Both of the results agree with the analytic derivative in the leading term, but differ in the order of δ^2.

We can conclude that using the estimated b_1 formula, Eq B8, will result in a discontinuity in the derivative of f at the periodic boundary with the order of magnitude δ^2. In the cases that the mode number M is very small compared to the grid points ($N = 2n$), the two methods should be very similar, but when some high M modes become important, the error from the second method can be significant.