Notes on Natural Cubic Splines
CSCI/MATH 3180: Numerical Analysis

Jackson Cole

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1 Overview/Quick Reference

Given data points (t_i, y_i), $0 \leq i \leq n$, the natural spline $S_i(x)$, defined for $[t_i, t_{i+1}]$ can be written as

$$S_i(x) = A_i + B_i(x - t_i) + C_i(x - t_i)^2 + D_i(x - t_i)^3 \tag{1}$$

We can then use Horner's algorithm to express equation (1) as

$$S_i(x) = A_i + (x - t_i)(B_i + (x - t_i)(C_i + (x - t_i)(D_i)))$$

We can then make the following definitions

$$h_i = t_{i+1} - t_i \qquad z_i = S''(t_i)$$

such that A_i, B_i, C_i, and D_i can be expressed as

$$\begin{aligned}
A_i &= y_i \\
B_i &= -\frac{h_i}{6} z_{i+1} - \frac{h_i}{3} z_i + \frac{(y_{i+1} - y_i)}{h_i} \\
C_i &= \frac{z_i}{2} \\
D_i &= \frac{z_{i+1} - z_i}{6h_i}
\end{aligned}$$

2 Outline of the derivation

1. Find a linear polynomial for $S_i''(x)$ using $z_i = S_i''(t_i)$.
2. Obtain $S_i(x)$ by integrating $S_i''(x)$ twice.
3. Convert $S_i(x)$ to another form to find coefficients easily.
   (a) Use $S_i'(t_i) = y_i$ and $S_i'(t_{i+1}) = y_{i+1}$ to determine the coefficients.
   (b) We have $S_i(x)$ now, but we don't know the z_is.
4. To find the values for z_is:
   (a) Differentiate $S_i(x)$ to obtain $S_i'(x)$.
   (b) Set $S_i'(t_i) = S_{i-1}'(t_i)$, which gives us a system of linear equations for the z_is.
   (c) Set $z_0 = z_n = 0$ for a natural cubic spline.
5. Convert $S_i(x)$ into a nested form for efficient evaluation.

3 Derivation of expression for the natural cubic spline

Step 1: Find a linear polynomial for $S_i''(x)$ using $z_i = S''(t_i)$.

We can assume that $S_i''(x)$ is a linear interpolant having (t_i, z_i) and (t_{i+1}, z_{i+1}) as endpoints. We can then find the Lagrange Interpolant for the two points, (t_i, z_i) and (t_{i+1}, z_{i+1}).

$$S_i''(x) = \left[\frac{(x - t_{i+1})}{(t_i - t_{i+1})}\right] z_i + \left[\frac{(x - t_i)}{(t_{i+1} - t_i)}\right] z_{i+1} \tag{2}$$

Now, if we let $h_i = t_{i+1} - t_i$, then we can write equation (2) as

$$S_i''(x) = \left[\frac{(x - t_{i+1})}{-h_i}\right] z_i + \left[\frac{(x - t_i)}{h_i}\right] z_{i+1} \tag{3}$$

We can then rewrite equation (3) as

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

Step 2: Obtain $S_i(x)$ by integrating $S_i''(x)$ twice.

In the last step, we obtained

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

If we integrate $S_i''(x)$, we get

$$S_i'(x) = \frac{z_{i+1}}{h_i}\left[\frac{1}{2}(x - t_i)^2\right] + \frac{z_i}{-h_i}\left[\frac{1}{2}(t_{i+1} - x)^2(-1)\right] + c$$

Integrating again gives us

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

which can then be rearranged a bit to give us

$$S_i(x) = \frac{z_{i+1}}{6h_i}(x - t_i)^3 + \frac{z_i}{6h_i}(t_{i+1} - x)^3 + cx + d \tag{4}$$

Step 3: Convert $S_i(x)$ into a nested form for efficient evaluation.

Note: I'm not actually entirely sure of the method by which equation (4) gets converted into equation (5), but I will just copy this line from the handout and move along.

$$S_i(x) = \frac{z_{i+1}}{6h_i}(x - t_i)^3 + \frac{z_i}{6h_i}(t_{i+1} - x)^3 + C(x - t_i) + D(t_{i+1} - x) \tag{5}$$

We can then use the boundary conditions that

$$S_i(t_i) = y_i \quad \text{and} \quad S_i(t_{i+1}) = y_{i+1}$$

so that we can find expressions for the coefficients, C_i, and D_i. Using this first condition gives us

$$\begin{aligned} S_i(t_i) &= y_i \\ &= \frac{z_{i+1}}{6h_i}(t_i - t_i)^3 + \frac{z_i}{6h_i}(t_{i+1} - t_i)^3 + C_i(t_i - t_i) + D_i(t_{i+1} - t_i) = y_i \\ &= \frac{z_i}{6h_i}(t_{i+1} - t_i)^3 + D_i(t_{i+1} - t_i) = y_i \end{aligned}$$

And given that $h_i = t_{i+1} - t_i$

$$\begin{aligned} \frac{z_i}{6h_i}h_i^3 + D_i h_i &= y_i \\ \frac{z_i}{6}h_i^2 + D_i h_i &= y_i \\ D_i h_i &= y_i - \frac{z_i}{6}h_i^2 \\ D_i &= \frac{y_i}{h_i} - \frac{z_i}{6}h_i \end{aligned}$$

Therefore, we can say

$$\boxed{D_i = \frac{y_i}{h_i} - \frac{z_i}{6}h_i}$$

Now, we can set about finding an expression for C_i. Using the second condition, we get

$$\begin{aligned}
S_i\left(t_{i+1}\right) &= \frac{z_{i+1}}{6h_i}\left(t_{i+1}-t_i\right)^3 + \frac{z_i}{6h_i}\left(t_{i+1}-t_{i+1}\right)^3 + C_i\left(t_{i+1}-t_i\right) + D\left(t_{i+1}-t_{i+1}\right) = y_{i+1} \\
&\to \frac{z_{i+1}}{6h_i}\left(t_{i+1}-t_i\right)^3 + C_i\left(t_{i+1}-t_i\right) = y_{i+1} \\
&\to \frac{z_{i+1}}{6h_i}h_i^3 + C_i h_i = y_{i+1} \\
&\to C_i h_i = y_{i+1} - \frac{z_{i+1}}{6h_i}h_i^3 \\
&\to C_i = \frac{y_{i+1}}{h_i} - \frac{z_{i+1}}{6}h_i
\end{aligned}$$

Therefore, we can say that

$$\boxed{C_i = \frac{y_{i+1}}{h_i} - \frac{z_{i+1}}{6}h_i}$$

Therefore, in terms of our new expressions for C_i and D_i, we can rewrite $S_i\left(x\right)$ as

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

Step 4: To find the values for z_is:

Differentiate $S_i\left(x\right)$ to obtain $S_i'\left(x\right)$

We first need to differentiate $S_i\left(x\right)$ to obtain $S_i'\left(x\right)$ in terms of the new expressions for the coefficients. This gives us

$$S_i'\left(x\right) = \frac{z_{i+1}}{2h_i}\left(x-t_i\right)^2 - \frac{z_i}{2h_i}\left(t_{i+1}-x\right)^2 + \left(\frac{y_{i+1}}{h_i} - \frac{z_{i+1}}{6}h_i\right) + -\left(\frac{y_i}{h_i} - \frac{z_i}{6}h_i\right)$$

Finding an expression for $S_{i-1}\left(x\right)$ and differentiating in the same way will give us $S_{i-1}'\left(x\right)$.

$$S_{i-1}'\left(x\right) = \frac{z_i}{2h_{i-1}}\left(x-t_{i-1}\right)^2 - \frac{z_{i-1}}{2h_{i-1}}\left(t_i-x\right)^2 + \left(\frac{y_i}{h_{i-1}} - \frac{z_i}{6}h_{i-1}\right) - \left(\frac{y_{i-1}}{h_{i-1}} - \frac{z_{i-1}}{6}h_{i-1}\right)$$

Notice that this expression is obtained from $S_{i-1}\left(x\right)$, which is just the expression for $S_i\left(x\right)$ with the subscripts shifted back.

Set $S_i'\left(t_i\right) = S_{i-1}'\left(t_i\right)$, which gives us a system of linear equations for the z_is

We can then make use of the condition that the first derivative of a natural cubic spline must be continuous. This condition allows us to say that

$$S_i'\left(t_i\right) = S_{i-1}'\left(t_i\right)$$

We can then proceed from this equation

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

Now, we can rewrite this last equation such that each term containing z has the form αz_i, where α is some coefficient.

$$
-\frac{h_i}{2}z_i - \frac{h_i}{6}z_{i+1} + \frac{h_i}{6}z_i + \frac{y_{i+1}}{h_i} - \frac{y_i}{h_i} \quad = \quad \frac{h_{i-1}}{2}z_i - \frac{h_{i-1}}{6}z_i + \frac{h_{i-1}}{6}z_{i-1} + \frac{y_i}{h_{i-1}} - \frac{y_{i-1}}{h_{i-1}}
$$

We can now move all terms containing z to the left-hand side, and all terms not containing z to the right-hand side.

$$
-\frac{h_i}{2}z_i - \frac{h_i}{6}z_{i+1} + \frac{h_i}{6}z_i - \frac{h_{i-1}}{2}z_i + \frac{h_{i-1}}{6}z_i - \frac{h_{i-1}}{6}z_{i-1} \quad = \quad +\frac{y_i}{h_{i-1}} - \frac{y_{i-1}}{h_{i-1}} - \frac{y_{i+1}}{h_i} + \frac{y_i}{h_i}
$$

Combining like terms gives us

$$
\begin{aligned}
-\frac{h_i}{2}z_i + \frac{h_i}{6}z_i - \frac{h_{i-1}}{2}z_i + \frac{h_{i-1}}{6}z_i - \frac{h_i}{6}z_{i+1} - \frac{h_{i-1}}{6}z_{i-1} \quad &= \quad -\frac{y_{i+1}}{h_i} + \frac{y_i}{h_i} + \frac{y_i}{h_{i-1}} - \frac{y_{i-1}}{h_{i-1}} \\
-\frac{3h_i}{6}z_i + \frac{h_i}{6}z_i - \frac{3h_{i-1}}{6}z_i + \frac{h_{i-1}}{6}z_i - \frac{h_i}{6}z_{i+1} - \frac{h_{i-1}}{6}z_{i-1} \quad &= \quad \frac{1}{h_i}(-y_{i+1} + y_i) + \frac{1}{h_{i-1}}(y_i - y_{i-1}) \\
-\frac{2h_i}{6}z_i - \frac{2h_{i-1}}{6}z_i - \frac{h_i}{6}z_{i+1} - \frac{h_{i-1}}{6}z_{i-1} \quad &= \quad \frac{1}{h_i}(-y_{i+1} + y_i) + \frac{1}{h_{i-1}}(y_i - y_{i-1}) \\
2h_iz_i + 2h_{i-1}z_i + h_iz_{i+1} + h_{i-1}z_{i-1} \quad &= \quad \frac{1}{6}\left[\frac{1}{h_i}(y_{i+1} - y_i) - \frac{1}{h_{i-1}}(y_i - y_{i-1})\right] \\
h_{i-1}z_{i-1} + 2(h_i + h_{i-1}) + h_iz_{i+1} \quad &= \quad \frac{1}{6}\left[\frac{1}{h_i}(y_{i+1} - y_i) - \frac{1}{h_{i-1}}(y_i - y_{i-1})\right]
\end{aligned}
$$

Set $z_0 = z_n = 0$ for a natural cubic spline

We can now consider the fact that at the left and right exterior points, the value of $S''(x) \equiv 0$. In our convention here, this is equivalent to setting $z_0 = z_n \equiv 0$. Then, we can make the following definitions

$$
u_i = 2(h_{i-1} + h_i) \quad \text{and} \quad v_i = \frac{1}{6}\left[\frac{1}{h_i}(y_{i+1} - y_i) - \frac{1}{h_{i-1}}(y_i - y_{i-1})\right]
$$

At this point, our definitions allow us to populate a system of linear equations, which we can then solve by other means.

$$\begin{array}{ccccccc}
h_0 z_0 & + & u_1 z_1 & + & h_1 z_2 & = & v_1 \\
h_1 z_1 & + & u_2 z_2 & + & h_2 z_3 & = & v_2 \\
h_2 z_2 & + & u_3 z_3 & + & h_3 z_4 & = & v_2 \\
\vdots & & \vdots & & \vdots & & \vdots \\
h_{n-2} z_{n-2} & + & u_{n-1} z_{n-1} & + & h_{n-1} z_n & = & v_{n-1}
\end{array}$$

If we notice the shifting indices, it should be clear that this can naturally be expressed as a tridiagonal system of equations, which can then be solved efficiently with tridiagonal methods.

Step 5: Convert $S_i(x)$ into a nested form for efficient evaluation.

We should first express $S_i(x)$ using Horner's algorithm, which we showed earlier in this derivation.

$$S_i(x) = A_i + (x - t_i)(B_i + (x - t_i)(C_i + (x - t_i)(D_i)))$$

The reason for doing this is not purely for computational efficiency, but also for allowing us to have a more convenient form to work with in this next step.

If we perform a Taylor expansion of $S_i(x)$ about t_i, we get that

$$S_i(x) = S_i(t_i) + S_i'(t_i)(x - t_i) + \frac{S_i''(t_i)}{2!}(x - t_i)^2 + \frac{S_i'''(t_i)}{3!}(x - t_i)^3$$

Actually, the form mentioned before isn't super helpful in this context. The assumed form of the cubic spline is

$$S_i(x) = A_i + B_i(x - t_i) + C_i(x - t_i)^2 + D_i(x - t_i)^3$$

Now, we can see that

$$A_i = S_i(t_i) \qquad B_i = S_i'(t_i) \qquad C_i = \frac{S_i''(t_i)}{2!} \qquad D_i = \frac{S_i'''(t_i)}{3!}$$

Now solving for A_i:

$$\begin{aligned}
A_i &= S_i(t_i) \\
&= \frac{z_{i+1}}{6h_i}(t_i - t_i)^3 + \frac{z_i}{6h_i}(t_{i+1} - t_i)^3 + \left(\frac{y_{i+1}}{h_i} - \frac{z_{i+1}}{6}h_i\right)(t_i - t_i) + \left(\frac{y_i}{h_i} - \frac{z_i}{6}h_i\right)(t_{i+1} - t_i) \\
&= \frac{z_i}{6}h_i^2 + \left(\frac{y_i}{h_i} - \frac{z_i}{6}h_i\right)(h_i) \\
&= y_i
\end{aligned}$$

Now solving for B_i:

$$\begin{aligned}
B_i &= S_i'(t_i) \\
&= -\frac{h_i}{2}z_i - \frac{h_i}{6}z_{i+1} + \frac{h_i}{6}z_i + \frac{y_{i+1}}{h_i} - \frac{y_i}{h_i} \\
&= -\frac{h_i}{6}z_{i+1} + \frac{h_i}{6}z_i - \frac{3h_i}{6}z_i + \frac{y_{i+1} - y_i}{h_i} \\
&= -\frac{h_i}{6}z_{i+1} - \frac{2h_i}{6}z_i + \frac{y_{i+1} - y_i}{h_i} \\
&= -\frac{h_i}{6}z_{i+1} - \frac{h_i}{3}z_i + \frac{y_{i+1} - y_i}{h_i}
\end{aligned}$$

Now solving for C_i:

$$\begin{aligned}
C_i &= \left.\frac{S_i''(x)}{2!}\right|_{x=t_i} \\
&= \frac{1}{2}\left[\frac{d}{dx}\left[\frac{z_{i+1}}{2h_i}(x-t_i)^2 - \frac{z_i}{2h_i}(t_{i+1}-x)^2 + \left(\frac{y_{i+1}}{h_i} - \frac{z_{i+1}}{6}h_i\right) + - \left(\frac{y_i}{h_i} - \frac{z_i}{6}h_i\right)\right]\right]\Bigg|_{x=t_i} \\
&= \frac{1}{2}\left[\frac{z_{i+1}}{h_i}(x-t_i) + \frac{z_i}{h_i}(t_{i+1}-x)\right]\Bigg|_{x=t_i} \\
&= \frac{1}{2}\left[\frac{z_{i+1}}{h_i}(t_i-t_i) + \frac{z_i}{h_i}(t_{i+1}-t_i)\right] \\
&= \frac{1}{2}[z_i] \\
&= \frac{z_i}{2}
\end{aligned}$$

Now solving for D_i by taking the second derivative from solving for C_i and differentiating:

$$\begin{aligned}
D_i &= \frac{S_i'''(t_i)}{3!} \\
&= \frac{1}{6}\left[\frac{d}{dx}\left[\frac{z_{i+1}}{h_i}(x-t_i) + \frac{z_i}{h_i}(t_{i+1}-x)\right]\right]\Bigg|_{x=t_i} \\
&= \frac{1}{6}\left[\frac{z_{i+1}}{h_i} - \frac{z_i}{h_i}\right]\Bigg|_{x=t_i} \\
&= \frac{z_{i+1}-z_i}{6h_i}
\end{aligned}$$