Accuracy of Interpolation and Splines

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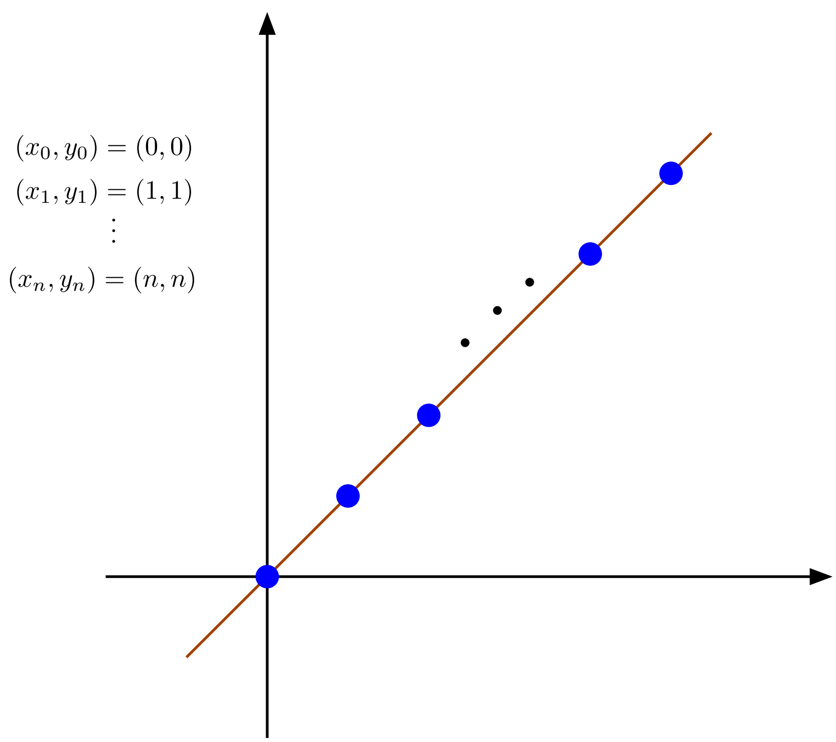
We saw three methods for polynomial interpolation (Vandermonde, Lagrange, Newton). It is important to understand that all three methods compute (in theory) the *same exact interpolant* $\mathcal{P}_n(x)$, just following different paths which may be better or worse from a computational perspective. The question however remains:

- How accurate is this interpolation, or in other words,
- How close is $\mathcal{P}_n(x)$ to the "real" function $f(x)$?

Example:



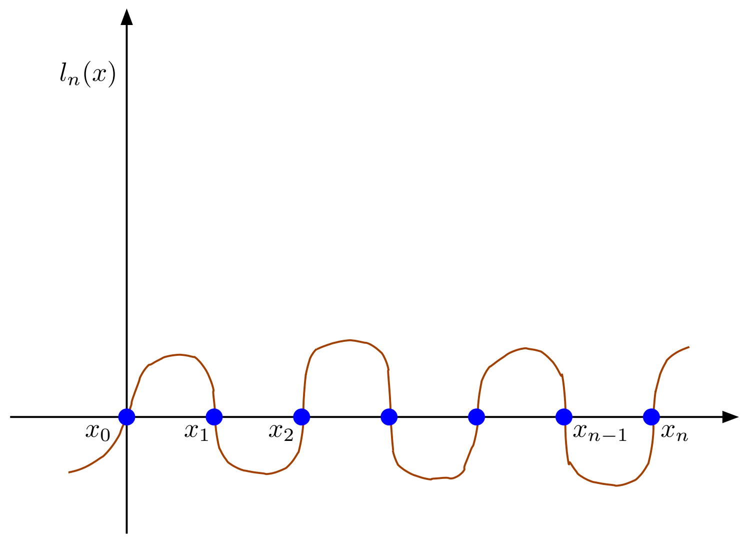
Using Lagrange polynomials $\mathcal{P}_n(x)$ $(= x)$ is written as

$$f(x) = \sum_{i=0}^{n} y_i l_i(x)$$

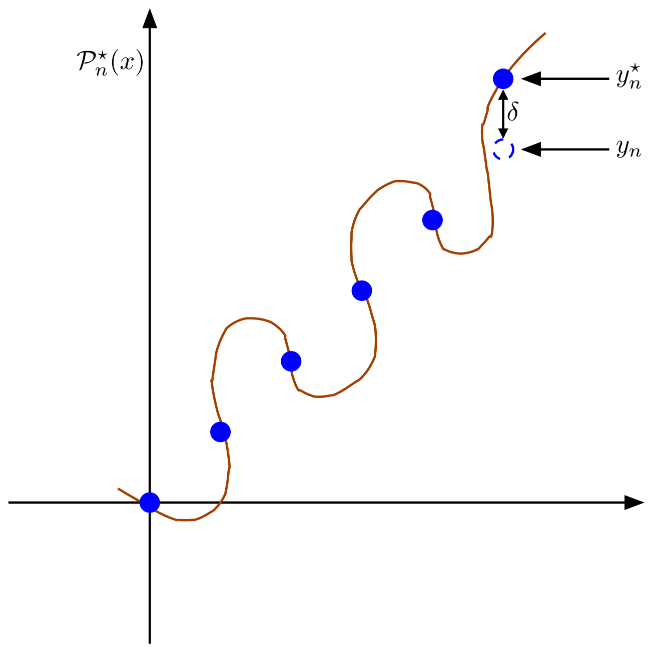
Let us "shift" y_n by a small amount δ. The new value is $y_n^\star = y_n + \delta$. The updated interpolant $\mathcal{P}_n^\star(x)$ then becomes:

$$\mathcal{P}_n^\star(x) = \sum_{i=0}^{n-1} y_i l_i(x) + y_n^\star l_n(x)$$

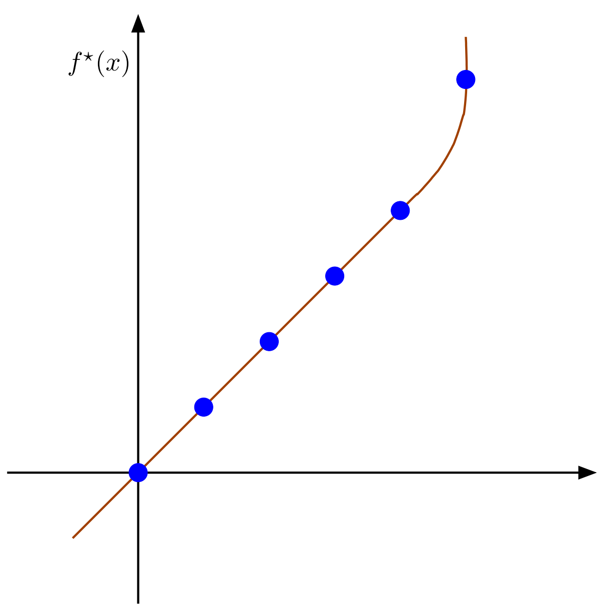
Thus, $\mathcal{P}_n^\star(x) - \mathcal{P}_n(x) = \delta \cdot l_n(x)$. Note that l_n is a function that "oscillates" through zero several times:



Thus, $\mathcal{P}_n^\star(x)$ looks like



What we observe is that a *local* change in y-values caused a *global* (and drastic) change in $\mathcal{P}_n(x)$. Perhaps the "real" function f would have exhibited a more graceful and localized change, e.g.:



We will use the following theorem to compare the "real" function f being sampled, and the reconstructed interpolant $\mathcal{P}_n(x)$.

Theorem 1. *Let*

- $x_0 < x_1 < \ldots < x_{n-1} < x_n$
- $y_n = f(x_n)$, $k = 0, 1, \ldots, n$, *where f is a function which is n-times differentiable with continuous derivatives*
- $\mathcal{P}_n(x)$ *is a polynomial that interpolates* $(x_0, y_0), (x_1, y_1) \ldots, (x_n, y_n)$

then for any $x \in (x_0, x_n)$, there exists a $\theta = \theta(x) \in (x_0, x_n)$ such that

$$f(x) - \mathcal{P}_n(x) = \frac{f^{(n+1)}(\theta)}{(n+1)!}(x - x_0)(x - x_1)\ldots(x - x_n)$$

This theorem may be difficult to apply directly since:

- θ is not known
- θ changes with x
- The $(n+1)$-th derivative $f^{(n+1)}(x)$ may not be fully known.

However, we can use it to derive a conservative bound:

Theorem 2. *If $M = \max_{x\in[x_0,x_n]} |f^{(n+1)}(x)|$ and $h = \max_{0\le i\le n} |x_{i+1} - x_i|$, then*

$$|f(x) - \mathcal{P}_n(x)| \le \frac{Mh^{n+1}}{4(n+1)}$$

for all $x \in [x_0, x_n]$.

How good is this, especially when we keep adding more and more data points (e.g., $n \to \infty$ and $h \to 0$), really depends on the higher order derivatives of $f(x)$. For example, $f(x) = \sin(x)$, $x \in [0, 2\pi]$, alll derivatives of f are $\pm\sin(x)$ or $\pm\cos(x)$. Thus, $|f^{(k)}(x)| \le 1$ for *any* k. In this case, $M = 1$, and as we add more (and denser) data points, we have

$$|f(x) - \mathcal{P}_n(x)| \le \frac{Mh^{n+1}}{4(n+1)} \xrightarrow[h\to 0]{n\to\infty} 0$$

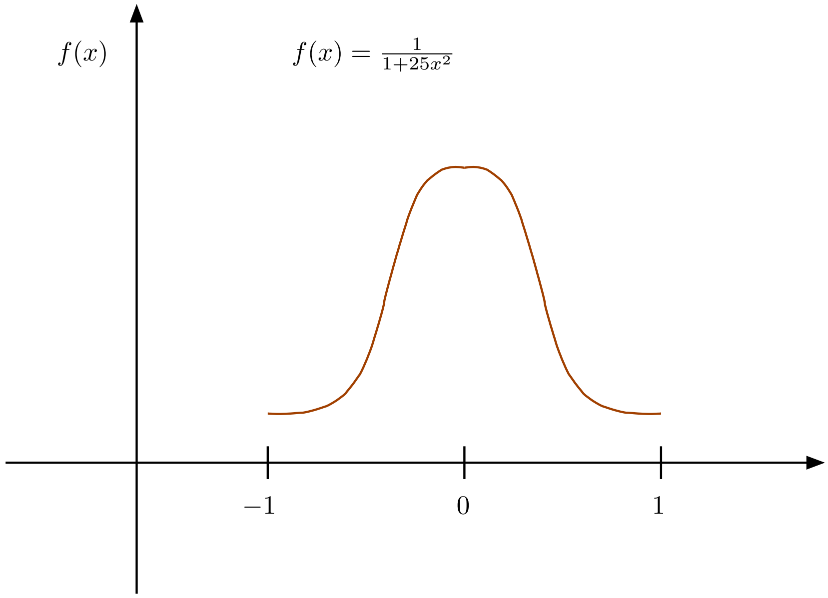
For some functions, however, the values of $|f^{(k)}(x)|$ grow vastly as $k \to \infty$ (i.e., when we introduce additional points). For example,

$$f(x) = \frac{1}{x}, \quad x \in (0.5, 1) \Rightarrow |f^{(n)}(x)| = n!\frac{1}{x^{n+1}}, M = \max_{x\in(0.5,1)} |f^{(n)}(x)| = n!2^{n+1}$$

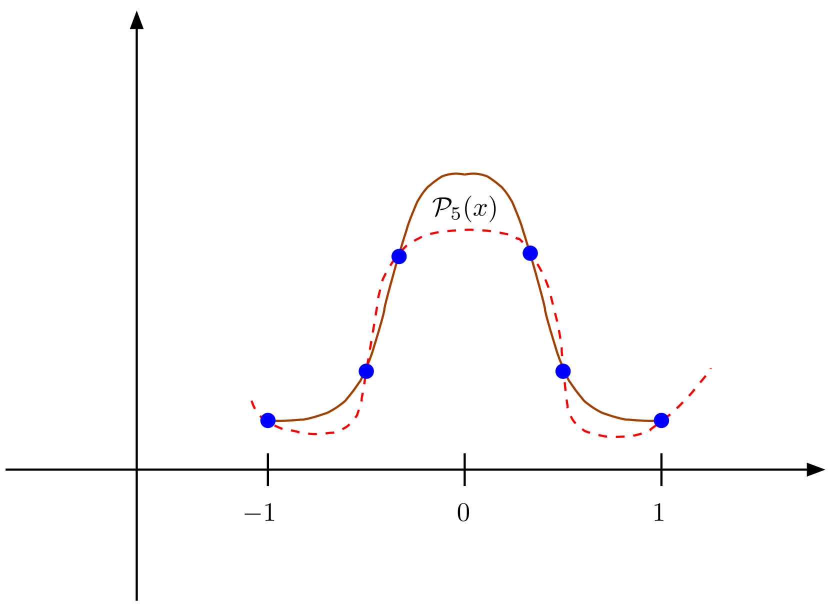
In this case, as $n \to \infty$:

$$\frac{Mh^n}{4n} = \frac{n!2^{n+1}h^n}{4n} \xrightarrow{n\to\infty} \infty$$

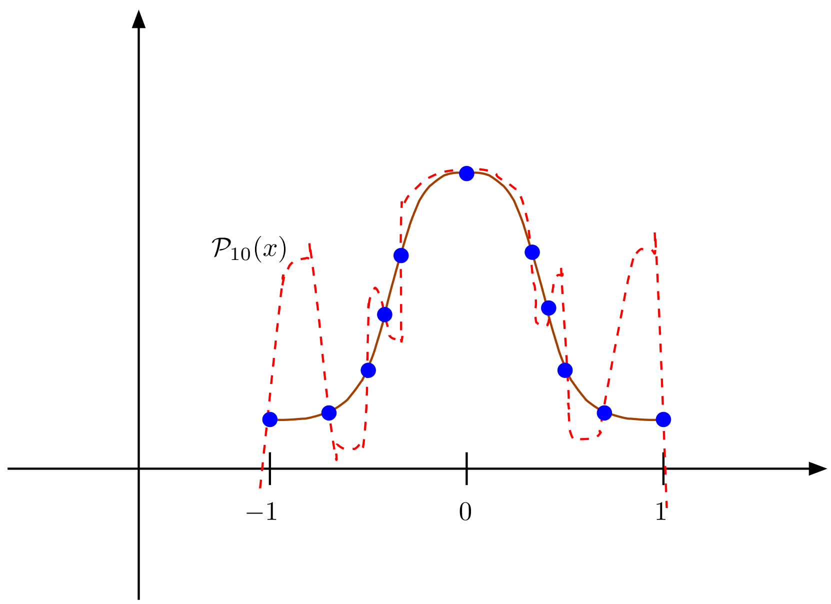
Another commonly cited example is *Runge's function*:



Approximation with a degree-5 polynomial:



Approximation with a degree-10 polynomial:



Thus, in this case, the polynomial $\mathcal{P}_k(x)$ do *not* uniformly converge to $f(x)$ as we add more points.

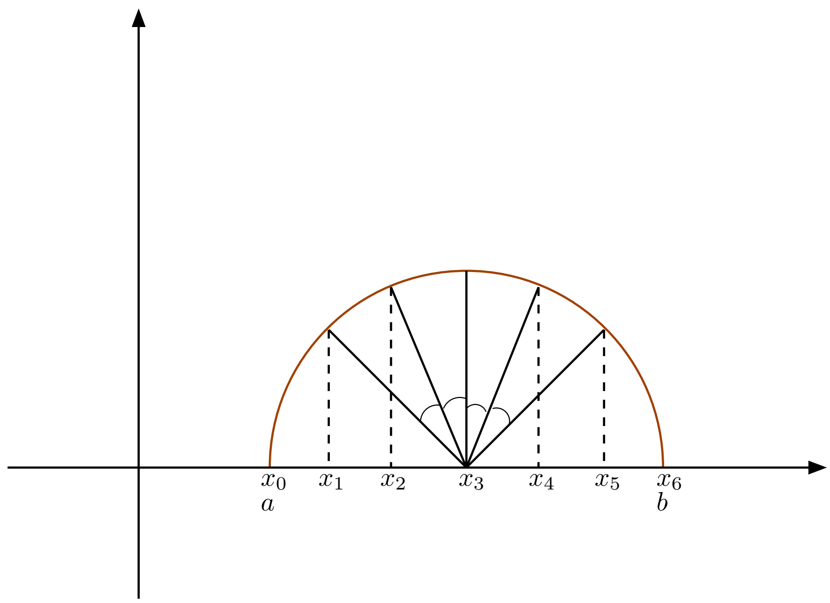
A possible improvement stems from the following idea:

$$f(x) - \mathcal{P}_n(x) = \underbrace{\frac{f^{(n+1)}(\theta)}{(n+1)!}}_{\text{this can be arbitrary}} \underbrace{(x - x_0)\dots(x - x_n)}_{\text{select points to minimize this product}}$$

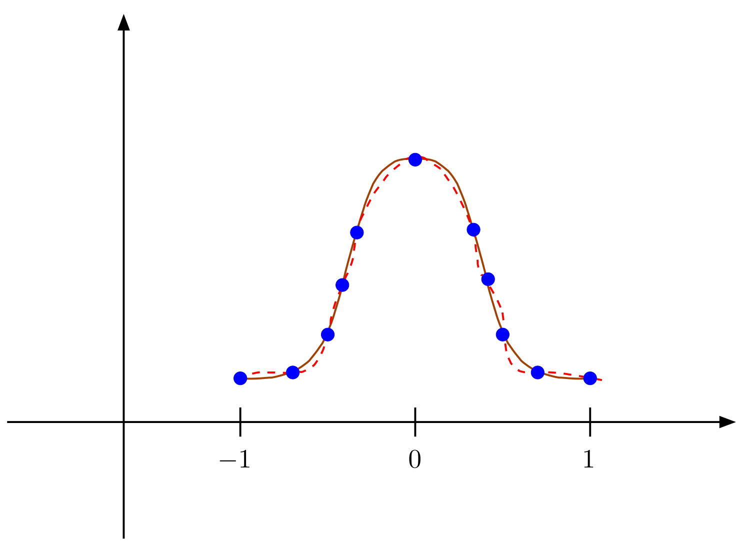
The value of the product $(x - x_0)\dots(x - x_n)$ is minimized by selecting the x_i's as the *Chebyshev points*. If the interpolation interval is $[a, b]$, the Chebyshev points are given by:

$$x_i = \frac{a+b}{2} + \frac{a-b}{2}\cos\left(\frac{i\pi}{n}\right), \quad i = 0, 1, 2, \dots, n$$

Graphically, these points are the projections on the x-axis of the $n+1$ points located along the half circle with diameter the interval $[a, b]$ at equal arc-lengths:



Now, we can re-try Runge's function using Chebyshev points:



In fact, it is possible to show that using Chebyshev points, we can guarantee that

$$|f(x) - \mathcal{P}_n(x)| \xrightarrow{n\to\infty} 0$$

provided that over $[a, b]$ both $f(x)$ and its derivative $f'(x)$ remain bounded (the benefit is that this condition does not place restrictions on higher-order derivatives of $f(x)$).

Although using Chebyshev points mitigates some of the drawbacks of high-order polynomial interpolants, this is still a non-ideal solution, since:

- We do not always have the flexibility to pick the x_i's.
- Polynomial interpolants of high degree typically require more than $O(n)$ computational cost to construct.
- Local changes in the data points affect the entire extent of the interpolant.

Piecewise Polynomials

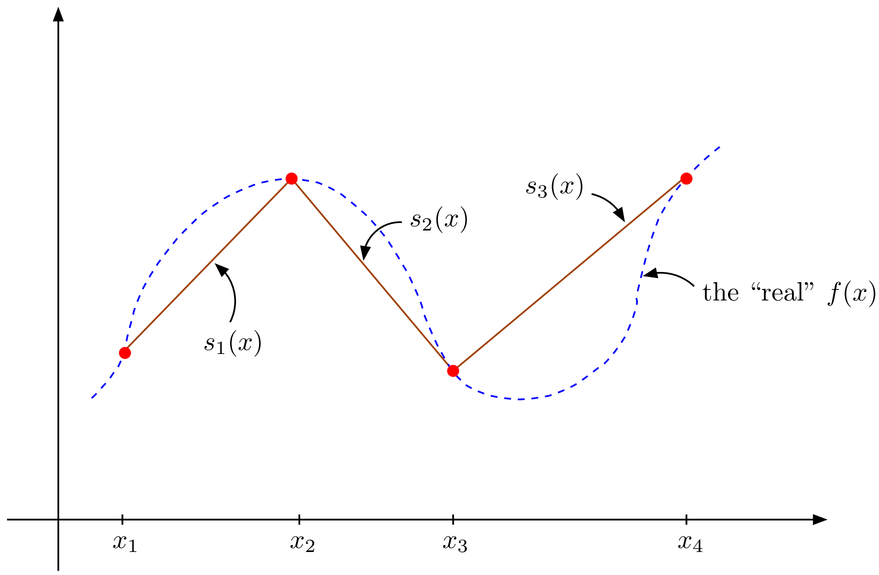
A better remedy is to use piecewise polynomials. Assume that the x-values $\{x_i\}_{i=1}^n$ are sorted in ascending order:

$$a = x_1 < x_2 < \ldots < x_n = b$$

Define $I_k = [x_k, x_{k+1}]$ and $h_k = |x_{k+1} - x_k|$. We also define the polynomials $s_1(x), s_2(x), \ldots, s_{n-1}(x)$ and use each of them to define the interpolant $s(x)$ at the respective interval I_k:

$$s(x) = \begin{cases} s_1(x), x \in I_1 \\ s_2(x), x \in I_2 \\ \vdots \\ s_{n-1}(x), x \in I_{n-1} \end{cases}$$

The benefit of using piecewise polynomial interpolants is that each $s_k(x)$ can be relatively low order and thus, non-oscillatory and easier to compute. The simplest piecewise polynomial interpolant is a *piecewise linear* curve:



In this case, every s_k can be written out explicitly as:

$$s_k(x) = y_k + \frac{y_{k+1} - y_k}{x_{k+1} - x_k}(x - x_k)$$

The next step is to examine the error $e(x) = f(x) - s_k(x)$ in the interval I_k. From the theorem we presented in the last lecture, we have that, for any $x \in I_k$ there is a $\theta_k = \theta(x_k) \in I_k$ such that:

$$e(x) = f(x) - s_k(x) = \frac{f''(\theta)}{2} \underbrace{(x - x_k)(x - x_{k+1})}_{q(x)} \tag{1}$$

We are interested in the *maximum* value of $|q(x)|$ in order to determine a bound for the error. $q(x)$ is a quadratic function which crosses zero at x_k and x_{k+1}, thus the extreme value is obtained at the midpoint $x_m = (x_k + x_{k+1})/2$. Thus,

$$|q(x)| \le |q(x_m)| = \left(\frac{x_{k+1} - x_k}{2}\right)^2 = \frac{h_k^2}{4}$$

for all $x \in I_k$. Using equation (1) gives:

$$\begin{aligned}
|f(x) - s_k(x)| &\le \max_{x\in I_k}\left|\frac{f''(x)}{2}\right| \cdot \max_{x\in I_k}|(x - x_k)(x - x_{k+1})| \\
&= \max_{x\in I_k}\left|\frac{f''(x)}{2}\right| \cdot \frac{h_k^2}{4} \\
\Rightarrow |f(x) - s_k(x)| &\le \frac{1}{8}\max_{x\in I_k}|f''(x)| \cdot h_k^2
\end{aligned}$$

for all $x \in I_k$.

Additionally, if we assume all data points are equally spaced, i.e.,

$$h_1 = h_2 = \ldots = h_{n-1} = h = \left(\frac{b-a}{n-1}\right)$$

we can additionally write:

$$|f(x) - s(x)| \leq \frac{1}{8} \max_{x \in [a,b]} |f''(x)| \cdot h^2$$

We often express the quantity on the right hand side using the "infinity norm" of a given function, defined as

$$||f||_\infty = \max_{x \in [a,b]} |f(x)|$$

Thus, using this notation:

$$\boxed{|f(x) - s(x)| \leq \frac{1}{8} ||f''||_\infty \cdot h^2}$$

Note that

- As $h \to 0$, the maximum discrepancy between f and s vanishes (proportionally to h^2)
- As we introduce more points, the quality of the approximation increases consistently, since the criterion above only considers the second derivative $f''(x)$ and not any higher order.

Piecewise cubic interpolation

In this approach, each $s_k(x)$ is a *cubic* polynomial, designed such that it interpolates the four data points:

$$(x_{k-1}, y_{k-1}), (x_k, y_k), (x_{k+1}, y_{k+1}), (x_{k+2}, y_{k+2})$$

As we will see, the benefit is that the error can be made even smaller than with piecewise linear curves; the drawback is that $s(x)$ can develop "kinks" (or corners) where two pieces s_k and s_{k+1} are joined.

Error of piecewise cubics:

$$f(x) - s_k(x) = \frac{f''''(\theta_k)}{4!} \underbrace{(x - x_{k-1})(x - x_k)(x - x_{k+1})(x - x_{k+2})}_{q(x)}$$

An analysis similar to the linear case can show that

$$|q(x)| \leq \frac{9}{16} \max\{h_{k-1}, h_k, h_{k+1}\}^4$$

If we again assume that $h_1 = h_2 = \ldots = h_{n-1} = h$, the error bound becomes:

$$\begin{aligned} |f(x) - s(x)| &\leq \frac{1}{24}||f''''||_\infty \frac{9}{16}h^4 \\ \Rightarrow |f(x) - s(x)| &\leq \frac{9}{384}||f''''||_\infty h^4 \end{aligned}$$

The next possibility we shall consider, is a piecewise cubic curve

$$s(x) = \begin{cases} s_1(x), x \in I_1 \\ s_2(x), x \in I_2 \\ \vdots \\ s_{n-1}(x), x \in I_{n-1} \end{cases}$$

where each $s_k(x) = a_3^{(k)}x^3 + a_2^{(k)}x^2 + a_1^{(k)}x + a_0^{(k)}$ and the coefficients $a_i^{(j)}$ are chosen as to *force* that the curve has continuous values, first and second derivatives:

$$\begin{aligned} s_k(x_{k+1}) &= s_{k+1}(x_{k+1}) \\ s'_k(x_{k+1}) &= s'_{k+1}(x_{k+1}) \\ s''_k(x_{k+1}) &= s''_{k+1}(x_{k+1}) \end{aligned}$$

The curve constructed this way is called a *cubic spline* interpolant.

The Cubic Spline

As always, our goal in this interpolation task is to define a curve $s(x)$ which interpolates the n data points

$$(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n) \quad \text{(where } x_1 < x_2 < \ldots < x_n\text{)}$$

In the fashion of piecewise polynomials, we will define $s(x)$ as a different cubic polynomial $s_k(x)$ at each sub-interval $I_k = [x_k, x_{k+1}]$, i.e.,

$$s(x) = \begin{cases} s_1(x), x \in I_1 \\ s_2(x), x \in I_2 \\ \vdots \\ s_{n-1}(x), x \in I_{n-1} \end{cases}$$

Each of the s_k's is a cubic polynomial:

$$s_k(x) = a_3^{(k)}x^3 + a_2^{(k)}x^2 + a_1^{(k)}x + a_0^{(k)}$$

where $a_3^{(k)}$, $a_2^{(k)}$, $a_1^{(k)}$, $a_0^{(k)}$ are unknown coefficients. Since we have $n-1$ piecewise polynomials, in total we shall have to determine $4(n-1) = 4n - 4$ unknown coefficients. The points $(x_2, x_3, \ldots, x_{n-1})$ where the formula for $s(x)$ changes from one cubic polynomial (s_k) to another (s_{k+1}) are called *knots*.

Note: In some textbooks, the extreme points x_1 and x_n are also included in the definition of what a knot is. We will stick with the definition we stated above.

The piecewise polynomial interpolation method described as *cubic spline* also requires the neighboring polynomials s_k and s_{k+1} to be joined at x_{k+1} with a certain degree of smoothness. In detail:

- The curve should be continuous: $s_k(x_{k+1}) = s_{k+1}(x_{k+1})$
- The derivative (slope) should be continuous: $s'_k(x_{k+1}) = s'_{k+1}(x_{k+1})$
- The 2nd derivative should be continuous as well: $s''_k(x_{k+1}) = s''_{k+1}(x_{k+1})$

(*Note:* If we force the next (3rd) derivative to match, this will force s_k and s_{k+1} to be exactly identical.)
When determining the unknown coefficients $\{a_i^{(j)}\}$, each of these 3 smoothness constraints (for knots $k = 2, 3, \ldots, n-1$) needs to be satisfied, for a total of $3(n-2) = 3n-6$ constraint equations. We should not forget that we additionally want to *interpolate* all n data points, i.e.,

$$s(x_i) = y_i \quad \text{for } i = 1, 2, \ldots, n$$

In total, we have $3n - 6 + n = 4n - 6$ total equations to satisfy, and $4n - 4$ unknowns! Consequently, we will need 2 more equations to ensure that the unknown coefficients will be uniquely determined. Several plausible options exist on how to do that:

1. The "not-a-knot" approach: We stipulate that at the locations of the first knot (x_2) and last knot (x_{n-1}) the *third* derivative of $s(x)$ should also be continuous, e.g.:

$$s'''_1(x_2) = s'''_2(x_2) \quad \text{and} \quad s'''_{n-2}(x_{n-1}) = s'''_{n-1}(x_{n-1})$$

   As we discussed before, these two additional constraints will effectively cause $s_1(x)$ to be identical with $s_2(x)$, and $s_{n-2}(x)$ to coincide with $s_{n-1}(x)$. In this sense, x_2 and x_{n-1} are no longer "knots" in the sense that the formula for $s(x)$ "changes" at these points (hence the name).

2. Complete spline: If we have access to the derivative f' of the function being sampled by the y_i's (i.e., $y_i = f(x_i)$), we can formulate the two additional constraints as:

$$s'_1(x_1) = f'(x_1) \quad \text{and} \quad s'_{n-1}(x_n) = f'(x_n)$$

   Note that qualitatively, using the complete spline approach is a better utilization of the flexibility of the spline curve in matching yet one more property of f. In contrast, the not-a-knot approach makes the spline "less flexible" by removing two degrees of freedom, in order to obtain a unique solution. However, we cannot always assume knowledge of f'.

3. The natural cubic spline: We use the following two constraints:

$$s''(x_1) = 0 \quad \text{and} \quad s''(x_n) = 0$$

   Thus, $s(x)$ reaches the endpoints looking like a straight line (instead of a curved one).

4. Periodic spline: The following two constraints are used:

$$s'(x_1) = s'(x_n) \quad \text{and} \quad s''(x_1) = s''(x_n)$$

   This is useful when the underlying function f is also known to be periodical over $[a, b]$.

Since $s(x)$ is piecewise cubic, its second derivative $s''(x)$ is piecewise linear on $[x_1, x_n]$. The linear Lagrange interpolation formula gives the following representation for $s''(x) = s''_k(x)$ on $[x_k, x_{k+1}]$:

$$s''_k(x) = s''(x_k)\frac{x - x_{k+1}}{x_k - x_{k+1}} + s''(x_{k+1})\frac{x - x_k}{x_{k+1} - x_k}$$

Defining $m_k = s''(x_k)$ and $h_k = x_{k+1} - x_k$ gives

$$s''_k(x) = \frac{m_k}{h_k}(x_{k+1} - x) + \frac{m_{k+1}}{h_k}(x - x_k)$$

for $x_k \leq x \leq x_{k+1}$ and $k = 1, 2, \ldots, n-1$. Integrating the above equation twice will introduce two constants of integration, and the result can be manipulated so that it has the form:

$$s_k(x) = \frac{m_k}{6h_k}(x_{k+1} - x)^3 + \frac{m_{k+1}}{6h_k}(x - x_k)^3 + p_k(x_{k+1} - x) + q_k(x - x_k) \tag{2}$$

Substituting x_k and x_{k+1} into equation (2) and using the values $y_k = s_k(x_k)$ and $y_{k+1} = s_k(x_{k+1})$ yields the following equations that involve p_k and q_k respectively:

$$y_k = \frac{m_k}{6}h_k^2 + p_k h_k \quad \text{and} \quad y_{k+1} = \frac{m_{k+1}}{6}h_k^2 + q_k h_k$$

These two equations are easily solved for p_k and q_k, and when these values are substituted into equation (2), the result is the following expression for the cubic function $s_k(x)$:

$$\begin{aligned} s_k(x) &= \frac{m_k}{6h_k}(x_{k+1} - x)^3 + \frac{m_{k+1}}{6h_k}(x - x_k)^3 + \left(\frac{y_k}{h_k} - \frac{m_k h_k}{6}\right)(x_{k+1} - x) \\ &+ \left(\frac{y_{k+1}}{h_k} - \frac{m_{k+1} h_k}{6}\right)(x - x_k) \end{aligned} \tag{3}$$

Notice that equation (3) has been reduced to a form that involves only the unknown coefficients $\{m_k\}$. To find these values, we must use the derivative of equation (3), which is

$$
\begin{aligned}
s'_k(x) &= -\frac{m_k}{2h_k}(x_{k+1}-x)^2 + \frac{m_{k+1}}{2h_k}(x-x_k)^2 - \left(\frac{y_k}{h_k} - \frac{m_k h_k}{6}\right) \\
&+ \frac{y_{k+1}}{h_k} - \frac{m_{k+1}h_k}{6} \qquad (4)
\end{aligned}
$$

Evaluating equation (4) at x_k and simplifying the result yields:

$$
s'_k(x_k) = -\frac{m_k}{3}h_k - \frac{m_{k+1}}{6}h_k + d_k, \quad \text{where } d_k = \frac{y_{k+1}-y_k}{h_k} \qquad (5)
$$

Similarly, we can replace k by $k-1$ in equation (4) to get the expression for $s'_{k-1}(x)$ and evaluate it at x_k to obtain

$$
s'_{k-1}(x_k) = \frac{m_k}{3}h_{k-1} + \frac{m_{k-1}}{6}h_{k-1} + d_{k-1} \qquad (6)
$$

Now using the continuity of derivatives and equations (5) and (6) gives an important relation involving m_{k-1}, m_k and m_{k+1}:

$$
h_{k-1}m_{k-1} + 2(h_{k-1}+h_k)m_k + h_k m_{k+1} = u_k \qquad (7)
$$

where $u_k = 6(d_k - d_{k-1})$ for $k = 2,\ldots,n-1$. Observe that the unknowns in equation (7) are the desired values $\{m_k\}$, and the other terms are constants obtained by performing simple arithmetic with the data points $\{x_k, y_k\}$. Therefore, in reality, system (7) is an underdetermined system of $n-2$ linear equations involving n unknowns. Hence, two additional equations must be supplied. They are used to eliminate m_1 and m_n. Consider the natural cubic spline strategy where m_1 and m_n are given ($=0$). The first equation (for $k=2$) of system (7) is:

$$
2(h_1+h_2)m_2 + h_2 m_3 = u_2 - h_1 m_1 \qquad (8)
$$

and similarly, the last equation is:

$$
h_{n-2}m_{n-2} + 2(h_{n-2}+h_{n-1})m_{n-1} = u_{n-1} - h_{n-1}m_n \qquad (9)
$$

Equations (8) and (9) with (7) used for $k = 3,4,\ldots,n-2$ form a tridiagonal $(n-2)\times(n-2)$ linear system $HM = V$ involving the coefficients $m_2, m_3, \ldots, m_{n-1}$:

$$
\begin{bmatrix}
b_2 & c_2 & & & & \\
a_3 & b_3 & c_3 & & & \\
 & & \ddots & & & \\
 & & & a_{n-3} & b_{n-2} & c_{n-2} \\
 & & & & a_{n-2} & b_{n-1}
\end{bmatrix}
\begin{bmatrix} m_2 \\ m_3 \\ \vdots \\ m_{n-2} \\ m_{n-1} \end{bmatrix}
=
\begin{bmatrix} v_2 \\ v_3 \\ \vdots \\ v_{n-2} \\ v_{n-1} \end{bmatrix}
$$

After the coefficients $\{m_k\}$ are determined, the spline coefficients $a_k^{(j)}$ for $s_k(x)$ are computed using the formulas

$$
a_k^{(0)} = y_k, \quad a_k^{(1)} = d_k - \frac{h_k}{6}(2m_k + m_{k+1}), \quad a_k^{(2)} = \frac{m_k}{2}, \quad a_k^{(3)} = \frac{m_{k+1}-m_k}{6h_k}
$$

Error analysis

For simplicity, we will again assume that

$$h_2 = h_3 = \ldots = h_{n-1} = h \qquad (h_k = x_{k+1} - x_k)$$

For the not-a-knot method, we have

$$|f(x) - s(x)| \lessapprox \frac{5}{384} ||f^{(4)}||_\infty \cdot h^4$$

The "approximate" inequality is used because the interpolation error can be slightly larger near the endpoints of the interval $[a, b]$. This is a very comparable result with the (non-smooth) piecewise cubic polynomial method:

$$|f(x) - s(x)| \leq \frac{9}{384} ||f^{(4)}||_\infty \cdot h^4$$

Note though that the computation of the piecewise cubic method was *very local* and simple (every interval could be independently evaluated) while the computation of the coefficients of the cubic spline is more elaborate.