Splines

Tuesday, September 22, 2020 1:17 PM

In our previous discussions of interpolation, we considered a single polynomial,

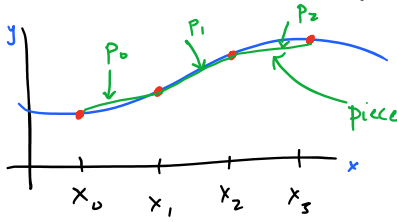
but if we have many points $\{x_0, x_1, \dots, x_n\}$, (we'll ALWAYS assume these are distinct) then we need a high-degree polynomial which can be undesirable (e.g., Runge phenomenon if equispaced nodes)

A very popular alternative is to do a piecewise polynomial interpolation

Ex: piecewise linear

The mathematics are straightforward so we won't focus on

p_i: polynomials
s is piecewise polynomial



$f(x)$ "underlying"/"true" function

piecewise linear interpolant $s = \begin{cases} p_1 & \text{if } x \in [x_0, x_1) \\ p_2 & x \in [x_1, x_2) \\ p_3 & x \in [x_2, x_3] \end{cases}$

In Matlab/numpy, this is "interp1"

Downside of piecewise linear is that the approximation is not differentiable, i.e., derivative on one piece doesn't match derivative on neighboring piece.

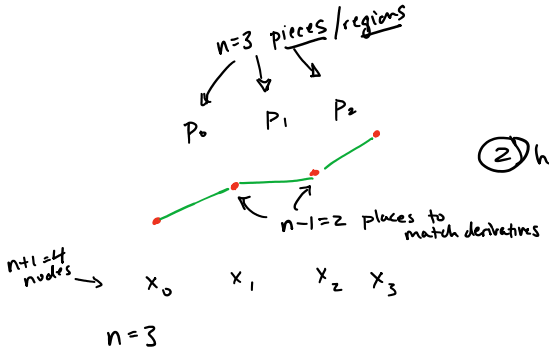
$s(x) = \{ p_j(x) \text{ if } x \in [x_j, x_{j+1}) \}$ i.e.,

① interpolation requirement $s(x_i) = f(x_i), \quad i = 0, 1, \dots, n$

meaning

$$p_i(x_i) = f(x_i)$$
$$p_i(x_{i+1}) = f(x_{i+1}) \quad i = 0, 1, \dots, n-1 \Big\} \; 2n \text{ constraints}$$

(So for n piecewise linear polynomials, we have $2n$ parameters, which matches $2n$ constraints ✓)



② have slopes agree on interior nodes $x_1, \dots, x_{n-1}$ (exclude x_0, x_n)

meaning

$$p_i'(x_{i+1}) = p_{i+1}'(x_{i+1}), \quad i = 0, 1, \dots, n-2 \Big\} \; n-1 \text{ constraints}$$

Going beyond linear interpolation,

what if we want to impose conditions ① and ②?

that's $2n + (n-1) = 3n-1$ constraints.

Suppose we use a quadratic rather than linear polynomial on each region?

Then $3n$ parameters but only $3n-1$ constraints so it's not unique unless we specify one more constraint. A boundary condition is natural, but only have room for one (x_0 or x_n, not both) ... AWKWARD!

Suppose we use a cubic polynomial? Then we have $4n$ parameters. We can add a lot of constraints. Let's add

(3) Have second derivatives agree on interior nodes

$$p_i''(x_{i+1}) = p_{i+1}''(x_{i+1}), \quad i = 0, 1, \ldots, n-2 \quad \Big\} \; n-1 \text{ constraints}$$

Then (1)+(2)+(3) is $2n + (n-1) + (n-1) = 4n-2$ constraints

So we have 2 extra degrees of freedom. This is a nice symmetric case. We can impose

(4') "Natural" or "Free" Boundaries,

$$S''(x_0) = 0 \qquad \text{i.e., no curvature at end}$$
$$S''(x_n) = 0 \qquad \text{i.e., } p_0''(x_0) = 0, \; p_{n-1}''(x_n) = 0$$

all useful. We'll focus on 4' "Natural"

OR

(4'') "clamped boundary" — of course only works if we can compute f'

$$S'(x_0) = f'(x_0) \qquad \text{i.e., } p_0'(x_0) = f'(x_0)$$
$$S'(x_n) = f'(x_n) \qquad p_{n-1}'(x_n) = f'(x_n)$$

OR

(4''') "not-a-knot"

S''' continuous at x_1 and x_{n-1}

i.e., $p_0'''(x_1) = p_1'''(x_1)$

$p_{n-2}'''(x_{n-1}) = p_{n-1}'''(x_{n-1})$

or (4'''') "periodic"

$S(x_0) = S(x_n)$

$S'(x_0) = S'(x_n)$

etc.

⚠ Condition (2) says $S \in C^1([a,b])$, i.e., derivatives match each other

Not the same as piecewise Hermite interpolation, which would require derivatives of S to match those of f

Conditions (1)+(2)+(3)+((4') or (4''')) do not require knowing f'

SPLINES

A piecewise function satisfying conditions like (1), (2) and (3) is called a spline.

(Note: B-Splines are a bit different, since don't interpolate, but have advantage that if you move a node, you don't have to recompute from scratch. Used in NURBS for CAD (computer-aided design) programs

These and Bézier curves (used in graphics, eg. fonts, vector graphics)

are beyond the scope of this course)

vector vs. raster (JPEG)
(no resolution)

We'll talk exclusively about CUBIC SPLINES ① + ② + ③ + ④

and in particular NATURAL CUBIC SPLINES ① + ② + ③ + ④'

⚠ interp1 (Matlab and Scipy) takes a "cubic" option but doesn't satisfy ③.

To get a cubic spline, scipy.interpolate.CubicSpline (all boundary conditions) (python)

or interp1 w/ "spline" option } "not-a-knot" (Matlab)
or spline
or csape / csapi (Matlab curve-fitting toolbox)

So... we have $3n$ degrees of freedom, $3n$ constraints

Basic technique: Fix a basis (representation) for the polynomials in each interval, setup a $3n \times 3n$ linear system, and solve in $O(n^3)$ time.

Tricks: pick a good representation for the polynomials (for stability) and tricks to solve system in $O(n)$ time

1) How to represent $p_j(x)$

ex. $p_j(x) = a_j + b_j x + c_j x^2 + d_j x^3$ $\quad j = 0, 1, \dots, n-1$

better: $p_j(x) = a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3$

2) Setup matrix system

$\Rightarrow \boxed{a_j = f(x_j)}$ ✓ (*)

Recall:

① 1a) $p_j(x_j) = f(x_j)$
1b) $p_j(x_{j+1}) = f(x_{j+1})$ $\quad j = 0, 1, \dots, n-1$

② $p_j'(x_{j+1}) = p_{j+1}'(x_{j+1})$ $\quad j = 0, 1, \dots, n-2$

③ $p_j''(x_{j+1}) = p_{j+1}''(x_{j+1})$ $\quad j = 0, 1, \dots, n-2$

④' $p_0''(x_0) = 0$
$p_{n-1}''(x_n) = 0$

Note $p_j'(x) = b_j + 2c_j(x - x_j) + 3d_j(x - x_j)^2$, $p_j''(x) = 2c_j + 6d_j(x - x_j)$

so $p_j'(x_j) = b_j$ (**) and likewise $p_j''(x_j) = 2c_j$ (***)

Notation: $h_j = \Delta x_j$, i.e., $h_j = x_{j+1} - x_j$

Note 1b can now be written $p_j(x_{j+1}) = f(x_{j+1}) = p_{j+1}(x_{j+1})$

$j = 0, 1, \dots, n-1$ (A) $a_j + b_j h_j + c_j h_j^2 + d_j h_j^3 = a_{j+1}$ $j = 0, 1, \dots, n-1$

via (*) (w/ $a_n := f(x_n)$)

And (2), with (**), gives $p_j'(x_{j+1}) = p_{j+1}'(x_{j+1})$

$j = 0, 1, \dots, n-1$ (B) $b_j + 2c_j h_j + 3d_j h_j^2 = b_{j+1}$ via (**) (w/ $b_n = s'(x_n)$)

And (3), with (***), gives $p_j''(x_{j+1}) = p_{j+1}''(x_{j+1})$

$j = 0, 1, \dots, n-1$ $2c_j + 6d_j h_j = 2c_{j+1}$ via (***) (w/ $c_n = s''(x_n)/2$)

i.e., (C) $c_j + 3d_j h_j = c_{j+1}$

$\Rightarrow d_j = \dfrac{c_{j+1} - c_j}{3h_j}$

Plug into

$j = 0, 1, \dots, n-1$

(A) $a_{j+1} = a_j + b_j h_j + h_j^2/3 (2c_j + c_{j+1})$

and

(B) $b_{j+1} = b_j + h_j (c_j + c_{j+1})$

Recall a_j are known!

1! you don't need to be able to recreate this on an exam

So $b_j = \frac{1}{h_j}(a_{j+1} - a_j) - h_j/3 (2c_j + c_{j+1})$ $(j = 0, 1, 2, \dots, n-1)$

and $b_{j+1} = \frac{1}{h_{j+1}}(a_{j+2} - a_{j+1}) - \frac{h_{j+1}}{3}(2c_{j+1} + c_{j+2})$ $(j = -1, 0, 1, \dots, n-2)$

* both hold for $j = 0, \dots, n-2$

So now (B) becomes (after grouping terms)

* $j = 0, 1, \dots, n-2$ $h_j c_j + 2(h_j + h_{j+1}) c_{j+1} + h_{j+1} c_{j+2} = \underbrace{\frac{3}{h_{j+1}}(a_{j+2} - a_{j+1}) - \frac{3}{h_j}(a_{j+1} - a_j)}_{\text{known!}}$

So... Solve these $(n-1)$ equations for c

then plug into earlier equations to find b and d.

Also need boundary condition (4') $p_0''(x_0) = 0$ and $p_{n-1}''(x_n) = 0$

$p_i''(x) = 2c_i + 6d_i(x - x_i)$

So $p_0''(x_0) = 2c_0$, so $p_0''(x_0) = 0$ means $c_0 = 0$.

also, recall we defined $c_n = s''(x_n)/2$, so $s''(x_n) = 0 \Rightarrow c_n = 0$.

Thus:

$$
\begin{aligned}
c_0 &= 0 &&\equiv y_0\\
h_0 c_0 + 2(h_0+h_1)c_1 + h_1 c_2 &= \tfrac{3}{h_1}(a_2-a_1) - \tfrac{3}{h_0}(a_1-a_0) &&\equiv y_1\\
h_1 c_1 + 2(h_1+h_2)c_2 + h_2 c_3 &= \tfrac{3}{h_2}(a_3-a_2) - \tfrac{3}{h_1}(a_2-a_1) &&\equiv y_2\\
&\vdots\\
h_{n-2}c_{n-2} + 2(h_{n-2}+h_{n-1})c_{n-1} + h_n c_n &= \tfrac{3}{h_{n-1}}(a_n-a_{n-1}) - \tfrac{3}{h_{n-2}}(a_{n-1}-a_{n-2}) &&\equiv y_n\\
c_n &= 0 &&\equiv y_n
\end{aligned}
$$

$$
\begin{bmatrix}
1 & 0 & 0 & 0 & \cdots & 0\\
h_0 & 2(h_0+h_1) & h_1 & 0 & & \vdots\\
0 & h_1 & 2(h_1+h_2) & h_2 & \ddots & \\
\vdots & & \ddots & \ddots & h_{n-1} & 0\\
 & & & h_{n-2} & 2(h_{n-2}+h_{n-1}) & h_{n-1}\\
0 & \cdots & & 0 & 0 & 1
\end{bmatrix}
\cdot
\begin{bmatrix} c_0\\ c_1\\ c_2\\ \vdots\\ c_{n-1}\\ c_n \end{bmatrix}
=
\begin{bmatrix} y_0\\ y_1\\ y_2\\ \vdots\\ y_{n-1}\\ y_n \end{bmatrix}
$$

This is a system of $(n+1)$ unknowns and $(n+1)$ equations

① Fact: it's invertible

(proof: it's "diagonally dominant", cf. ch 6.6, and by the Gershgorin Disk theorem, there are
aka Gershgorin Circle
no eigenvalues ... a special case is proven in Thm. 6.21)

② It's a tridiagonal matrix, and can be solved efficiently

A fact* everyone should know

Specifically, note that solving a general system of n linear equations and n unknowns takes $O(n^3)$ flops

$$\underbrace{\boxed{A}}_{n\times n}\,[x] = [b]$$

* it's not quite true due to fast Strassen based schemes, but it's true enough

But if you know A is diagonal, now it's uncoupled, so only $O(n)$ flops

$$\boxed{\diagdown}\,[x] = [b]$$

If it's lower (or upper triangular), it's $O(n^2)$ flops

It turns out tridiagonal matrices can be solved in $O(n)$ flops, e.g. "Thomas Algorithm" or "Crout Factorization" (Algo 6.7 in our book)

in Matlab/Scipy, using a sparse structure will already make it pretty fast to solve

Theory

Thm 3.11 There is a unique natural (4') cubic spline interpolant

proof we just proved this when we showed the above tridiagonal matrix is invertible

Thm 3.12 If f is differentiable at x_0 and x_n, then there is a unique clamped (4'') cubic spline interpolant

proof similar

Error Bounds

Thm 3.13 If $f \in C^4([a,b])$ with $\max_{x\in[a,b]} |f^{(4)}(x)| = M$ and

S is the clamped cubic spline interpolant on

$a = x_0 < x_1 < x_2 < \dots < x_n = b$ then

$$(\forall\, x \in [a,b]) \quad |f(x) - S(x)| \le M \cdot \frac{5}{384} \cdot \max_{0\le j\le n-1} (x_{j+1} - x_j)^4.$$

(similar results hold for natural and not-a-knot cubic splines)

Interpretation of Thm 3.13

Consider uniformly spaced points

$$x_0 = a, \quad x_1 = a+h, \quad x_2 = a+2h, \quad \dots, \quad x_n = a + nh = b$$

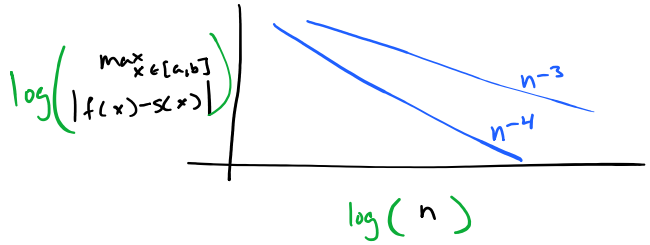
so $h = \frac{b-a}{n}$

then the theorem says the error is

$$|f(x) - S(x)| \le \text{constant} \cdot h^4$$

i.e. $\le$ constant $\cdot\, n^{-4}$

We say it is **4th order accurate**



$y = n^{\alpha}$ is a straight-line on a log-log plot

top 10 fact you should know after this course

Summary

Cubic Splines are piece-wise cubic, C^2 functions that interpolate on the nodes, are 4th order accurate, and require $O(n)$ computation for $n+1$ nodes.