CMPSC/Math 451, Numerical Computation

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Introduction

Disadvantages of polynomial interpolation $P_n(x)$

- n-time differentiable. We do not need such high smoothness;
- big error in certain intervals (esp. near the ends);
- no convergence result;
- Heavy to compute for large n

Suggestion: use piecewise polynomial interpolation.

Usage:

- visualization of discrete data
- graphic design

Requirement:

- interpolation
- certain degree of smoothness

Problem setting

Given a set of data

x	t_0	t_1	$\cdots$	t_n
y	y_0	y_1	$\cdots$	y_n

Find a function $\mathcal{S}(x)$ which interpolates the points $(t_i, y_i)_{i=0}^n$.

The set $t_0 < t_1 < \cdots < t_n$ are called knots. Note that they need to be ordered.

$\mathcal{S}(x)$ consists of piecewise polynomials

$$\mathcal{S}(x) \doteq \begin{cases} \mathcal{S}_0(x), & t_0 \le x \le t_1 \\ \mathcal{S}_1(x), & t_1 \le x \le t_2 \\ \vdots & \\ \mathcal{S}_{n-1}(x), & t_{n-1} \le x \le t_n \end{cases}$$

Definition for a spline of degree k

$\mathcal{S}(x)$ is called *a spline of degree* k, if

- $\mathcal{S}_i(x)$ is a polynomial of degree k;
- $\mathcal{S}(x)$ is $(k-1)$ times continuous differentiable, i.e., for $i = 1, 2, \cdots, k-1$ we have

$$
\begin{aligned}
\mathcal{S}_{i-1}(t_i) &= \mathcal{S}_i(t_i), \\
\mathcal{S}'_{i-1}(t_i) &= \mathcal{S}'_i(t_i), \\
&\vdots \\
\mathcal{S}^{(k-1)}_{i-1}(t_i) &= \mathcal{S}^{(k-1)}_i(t_i),
\end{aligned}
$$

Commonly used splines:

- $k = 1$: linear spline (simplest)
- $k = 2$: quadratic spline (less popular)
- $k = 3$: cubic spline (most used)

Example 1. Determine whether this function is a first-degree spline function:

$$S(x) = \begin{cases} x & x \in [-1, 0] \\ 1 - x & x \in (0, 1) \\ 2x - 2 & x \in [1, 2] \end{cases}$$

Answer. Check all the properties of a linear spline.

- Linear polynomial for each piece: OK.
- $S(x)$ is continuous at inner knots:
  At $x = 0$, $S(x)$ is discontinuous, because from the left we get 0 and from the right we get 1.

Therefore this is NOT a linear spline.

Example 2. Determine whether the following function is a quadratic spline:

$$S(x) = \begin{cases} x^2 & x \in [-10, 0] \\ -x^2 & x \in (0, 1) \\ 1 - 2x & x \geq 1 \end{cases}$$

Answer. Let's label each piece:

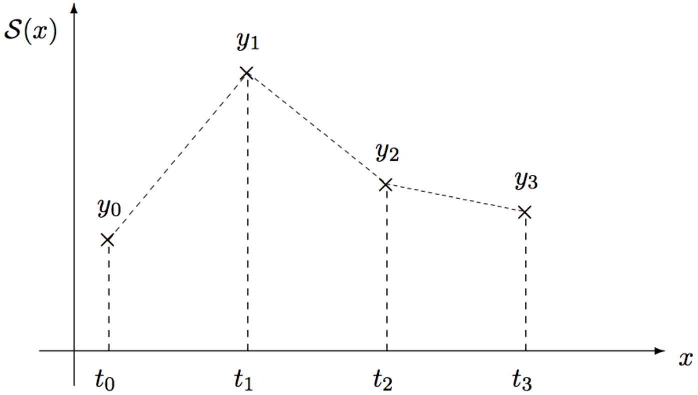
$$Q_0(x) = x^2, \quad Q_1(x) = -x^2, \quad Q_2(x) = 1 - 2x.$$

We now check all the conditions, i.e, the continuity of Q and Q' at inner knots $0, 1$:

$$\begin{aligned} Q_0(0) = 0, &\quad Q_1(0) = 0, &\qquad \text{OK} \\ Q_1(1) = -1, &\quad Q_2(1) = -1, &\qquad \text{OK} \\ Q_0'(0) = 0, &\quad Q_1'(0) = 0, &\qquad \text{OK} \\ Q_1'(1) = -2, &\quad Q_2'(1) = -2, &\qquad \text{OK} \end{aligned}$$

It passes all the test, so it is a quadratic spline.

$n = 1$: piecewise linear interpolation, i.e., straight line between 2 neighboring points.



Requirements:

$$\begin{aligned}
\mathcal{S}_0(t_0) &= y_0 \\
\mathcal{S}_{i-1}(t_i) = \mathcal{S}_i(t_i) &= y_i, \qquad i = 1, 2, \cdots, n-1 \\
\mathcal{S}_{n-1}(t_n) &= y_n.
\end{aligned}$$

Easy to find: write the equation for a line through two points: (t_i, y_i) and (t_{i+1}, y_{i+1}),

$$\mathcal{S}_i(x) = y_i + \frac{y_{i+1} - y_i}{t_{i+1} - t_i}(x - t_i), \qquad i = 0, 1, \cdots, n-1.$$

Accuracy Theorem for linear spline:

Assume $t_0 < t_1 < t_2 < \cdots < t_n$, and let $h_i = t_{i+1} - t_i$, $h = \max_i h_i$.

$f(x)$: given function, $\mathcal{S}(x)$: a linear spline

$$\mathcal{S}(t_i) = f(t_i), \qquad i = 0, 1, \cdots, n$$

We have the following, for $x \in [t_0, t_n]$,

(1) If f'' exits and is continuous, then

$$|f(x) - \mathcal{S}(x)| \le \max_i \left\{ \frac{1}{8} h_i^2 \max_{t_i \le x \le t_{i+1}} |f''(x)| \right\} \le \frac{1}{8} h^2 \max_x |f''(x)| \,.$$

(2) If f' exists and is continuous, then

$$|f(x) - \mathcal{S}(x)| \le \max_i \left\{ \frac{1}{2} h_i \max_{t_i \le x \le t_{i+1}} |f'(x)| \right\} \le \frac{1}{2} h \max_x |f'(x)| \,.$$

To minimize error, it is obvious that one should add more knots where the function has large first or second derivative.

Quadratic spline: Self study.

Natural cubic spline

Given $t_0 < t_1 < \cdots < t_n$, we define the *cubic spline*, with

$$\mathcal{S}(x) = \mathcal{S}_i(x) \quad \text{for} \quad t_i \leq x \leq t_{i+1}$$

Write

$$\mathcal{S}_i(x) = a_i x^3 + b_i x^2 + c_i x + d_i, \qquad i = 0, 1, \cdots, n-1$$

Total number of unknowns$= 4 \cdot n$.

Requirements: $\mathcal{S}, \mathcal{S}', \mathcal{S}''$ are all continuous.

Equations we have

$$\left.\begin{array}{llll} & \text{equation} & & \text{number} \\ (1) & \mathcal{S}_i(t_i) = y_i, & i = 0, 1, \cdots, n-1 & n \\ (2) & \mathcal{S}_i(t_{i+1}) = y_{i+1}, & i = 0, 1, \cdots, n-1 & n \\ (3) & \mathcal{S}_i'(t_{i+1}) = \mathcal{S}_{i+1}'(t_{i+1}), & i = 0, 1, \cdots, n-2 & n-1 \\ (4) & \mathcal{S}_i''(t_{i+1}) = \mathcal{S}_{i+1}''(t_{i+1}), & i = 0, 1, \cdots, n-2 & n-1 \\ (5) & \mathcal{S}_0''(t_0) = 0, \mathcal{S}_{n-1}''(t_n) = 0, & & 2 \end{array}\right\} \text{total} = 4n.$$

How to compute $\mathcal{S}_i(x)$? We know:

$$\begin{array}{ccl} \mathcal{S}_i & : & \text{polynomial of degree 3} \\ \mathcal{S}_i' & : & \text{polynomial of degree 2} \\ \mathcal{S}_i'' & : & \text{polynomial of degree 1} \end{array}$$

Procedure:

- Start with $\mathcal{S}_i''(x)$, they are all linear, one can use Lagrange form,
- Integrate $\mathcal{S}_i''(x)$ twice to get $\mathcal{S}_i(x)$, you will get 2 integration constant
- Determine these constants. Various tricks on the way...

Natural Cubic Splines; Derivation of Algorithm

$$\text{Define:} \quad z_i = \mathcal{S}''(t_i), \qquad i = 1, 2, \cdots, n-1, \qquad z_0 = z_n = 0$$

NB! These z_i's are our unknowns.
Let $h_i = t_{i+1} - t_i$. Lagrange form for S_i'':

$$\mathcal{S}_i''(x) = \frac{z_{i+1}}{h_i}(x - t_i) - \frac{z_i}{h_i}(x - t_{i+1}).$$

Then

$$\begin{aligned}
\mathcal{S}_i'(x) &= \frac{z_{i+1}}{2h_i}(x - t_i)^2 - \frac{z_i}{2h_i}(x - t_{i+1})^2 + C_i - D_i \\
\mathcal{S}_i(x) &= \frac{z_{i+1}}{6h_i}(x - t_i)^3 - \frac{z_i}{6h_i}(x - t_{i+1})^3 + C_i(x - t_i) - D_i(x - t_{i+1}).
\end{aligned}$$

You can check by yourself that these $\mathcal{S}_i, \mathcal{S}_i'$ are correct.

Interpolating properties: (1). $\mathcal{S}_i(t_i) = y_i$ gives

$$y_i = -\frac{z_i}{6h_i}(-h_i)^3 - D_i(-h_i) = \frac{1}{6}z_i h_i^2 + D_i h_i \quad \Rightarrow \quad D_i = \frac{y_i}{h_i} - \frac{h_i}{6}z_i$$

(2). $\mathcal{S}_i(t_{i+1}) = y_{i+1}$ gives

$$y_{i+1} = \frac{z_{i+1}}{6h_i}h_i^3 + C_i h_i, \quad \Rightarrow \quad C_i = \frac{y_{i+1}}{h_i} - \frac{h_i}{6}z_{i+1}.$$

We see that, once z_i's are known, then (C_i, D_i)'s are known, and so $\mathcal{S}_i, \mathcal{S}_i'$ are known.

$$\begin{aligned}
\mathcal{S}_i(x) &= \frac{z_{i+1}}{6h_i}(x-t_i)^3 - \frac{z_i}{6h_i}(x-t_{i+1})^3 + \left(\frac{y_{i+1}}{h_i} - \frac{h_i}{6}z_{i+1}\right)(x-t_i) \\
&\quad - \left(\frac{y_i}{h_i} - \frac{h_i}{6}z_i\right)(x-t_{i+1}). \\
\mathcal{S}_i'(x) &= \frac{z_{i+1}}{2h_i}(x-t_i)^2 - \frac{z_i}{2h_i}(x-t_{i+1})^2 + \frac{y_{i+1}-y_i}{h_i} - \frac{z_{i+1}-z_i}{6}h_i.
\end{aligned}$$

Continuity of $\mathcal{S}'(x)$ requires

$$\mathcal{S}'_{i-1}(t_i) = \mathcal{S}'_i(t_i), \qquad i = 1, 2, \cdots, n-1$$

$$\begin{aligned}
\mathcal{S}'_i(t_i) &= -\frac{z_i}{2h_i}(-h_i)^2 + \underbrace{\frac{y_{i+1}-y_i}{h_i}}_{b_i} - \frac{z_{i+1}-z_i}{6}h_i \\
&= -\frac{1}{6}h_i z_{i+1} - \frac{1}{3}h_i z_i + b_i \\
\mathcal{S}'_{i-1}(t_i) &= \frac{1}{6}z_{i-1}h_{i-1} + \frac{1}{3}z_i h_{i-1} + b_{i-1}
\end{aligned}$$

Set them equal to each other, we get

$$\begin{cases} h_{i-1}z_{i-1} + 2(h_{i-1}+h_i)z_i + h_i z_{i+1} = 6(b_i - b_{i-1}), & i = 1, 2, \cdots, n-1 \\ z_0 = z_n = 0. \end{cases}$$

$$\begin{cases} h_{i-1}z_{i-1} + 2(h_{i-1} + h_i)z_i + h_i z_{i+1} = 6(b_i - b_{i-1}), & i = 1, 2, \cdots, n-1 \\ z_0 = z_n = 0. \end{cases}$$

In matrix-vector form: $\mathbf{H} \cdot \vec{z} = \vec{b}$

$$\mathbf{H} = \begin{pmatrix} 2(h_0 + h_1) & h_1 & & & & \\ h_1 & 2(h_1 + h_2) & h_2 & & & \\ & h_2 & 2(h_2 + h_3) & h_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & h_{n-3} & 2(h_{n-3} + h_{n-2}) & h_{n-2} \\ & & & & h_{n-2} & 2(h_{n-2} + h_{n-1}) \end{pmatrix}$$

$\mathbf{H}$: tri-diagonal, symmetric, and diagonal dominant

$$2\,|h_{i-1} + h_i| > |h_i| + |h_{i-1}|$$

which implies unique solution.

$$\begin{cases} h_{i-1}z_{i-1} + 2(h_{i-1}+h_i)z_i + h_i z_{i+1} = 6(b_i - b_{i-1}), & i = 1, 2, \cdots, n-1 \\ z_0 = z_n = 0. \end{cases}$$

$$\vec{z} = \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ \vdots \\ z_{n-2} \\ z_{n-1} \end{pmatrix}, \qquad \vec{b} = \begin{pmatrix} 6(b_1 - b_0) \\ 6(b_2 - b_1) \\ 6(b_3 - b_2) \\ \vdots \\ 6(b_{n-2} - b_{n-3}) \\ 6(b_{n-1} - b_{n-2}) \end{pmatrix}.$$

Summarizing the algorithm:

- Set up the matrix-vector equation and solve for z_i.
- Compute $S_i(x)$ using these z_i's.

See Matlab codes.

Theorem on smoothness of cubic splines.

Theorem. *If $\mathcal{S}$ is the natural cubic spline function that interpolates a twice-continuously differentiable function f at knots*

$$a = t_0 < t_1 < \cdots < t_n = b$$

then

$$\int_a^b \left[\mathcal{S}''(x)\right]^2 \, dx \le \int_a^b \left[f''(x)\right]^2 \, dx.$$

Note that $\int (f'')^2$ is related to the curvature of f.
Cubic spline gives the least curvature, $\Rightarrow$ most smooth, so best choice.

Proof. Let

$$g(x) = f(x) - \mathcal{S}(x)$$

Then

$$g(t_i) = 0, \qquad i = 0, 1, \cdots, n$$

and

$$f'' = \mathcal{S}'' + g'', \qquad (f'')^2 = (\mathcal{S}'')^2 + (g'')^2 + 2\mathcal{S}''g''$$

$$\Rightarrow \quad \int_a^b (f'')^2\,dx = \int_a^b (\mathcal{S}'')^2\,dx + \int_a^b (g'')^2\,dx + \int_a^b 2\mathcal{S}''g''\,dx$$

We claim that

$$\int_a^b \mathcal{S}''g''\,dx = 0$$

then this would imply

$$\int_a^b (f'')^2\,dx \geq \int_a^b (\mathcal{S}'')^2\,dx$$

and we are done.

Proof of the claim:

$$\int_a^b \mathcal{S}'' g''\, dx = 0$$

Using integration-by-parts,

$$\int_a^b \mathcal{S}'' g''\, dx = \mathcal{S}'' g' \Big|_a^b - \int_a^b \mathcal{S}''' g'\, dx$$

Since $S''(a) = S''(b) = 0$, the first term is 0.
For the second term, since $\mathcal{S}'''$ is piecewise constant. Call

$$c_i = \mathcal{S}'''(x), \quad \text{for} \quad x \in [t_i, t_{i+1}].$$

Then

$$\int_a^b \mathcal{S}''' g'\, dx = \sum_{i=0}^{n-1} c_i \int_{t_i}^{t_{i+1}} g'(x)\, dx = \sum_{i=0}^{n-1} c_i \left[g(t_{i+1}) - g(t_i) \right] = 0,$$

(b/c $g(t_i) = 0$).