AMSC/CMSC 460 Computational Methods, Fall 2007
UNIT 2: Spline Approximations
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Piecewise polynomial interpolation

Piecewise polynomial interpolation

Read: Chapter 3. Skip: 3.2.

So far, we can determine a polynomial that passes through a given set of data points.

Advantages of polynomial interpolation:

- Easy to compute the polynomial and evaluate it at a set of points.
- Have a theorem telling us how close we are to the function

Disadvantage of polynomial interpolation:

- Polynomials tend to oscillate (wiggle) a lot, even when our true function does not.

The plan for this unit:

- Piecewise linear interpolation
- Cubic splines

Piecewise linear interpolation

Piecewise linear interpolation

Problem: Given a set of data points $(x_1, y_1), \ldots, (x_n, y_n)$, pass a piecewise linear function through the data.

Picture

Let's call the points $x_1, \ldots, x_n$ knots and assume that
$a = x_1 < x_2 < \ldots < x_n = b$.

The formula for the piecewise linear function

We've already done all of the work in the previous chapter. Let's use the Lagrange basis to find the formula for the interpolant on the interval $[x_i, x_{i+1}]$:

$$p(x) = y_i \frac{x - x_{i+1}}{x_i - x_{i+1}} + y_{i+1} \frac{x - x_i}{x_{i+1} - x_i}\,, \quad i = 1, 2, \ldots, n-1\,.$$

Unquiz:

- What should we do if $x < x_1$ or $x > x_n$?
- What is the formula for $p'(x)$?
- Suppose we want to evaluate the interpolant at $x = .85$. Write code to decide which formula to use and then to evaluate that formula.

Evaluating the piecewise linear function

See `Locate` and `Lvals` on pp. 108-109. Pay special attention to the binary search algorithm, important in other problems, too.

How good is piecewise linear interpolation?

Recall from Polynomial interpolation: If $f \in \mathcal{C}^n[I]$, then

$$f(x) - p_{n-1}(x) = \frac{(x - x_1) \ldots (x - x_n) f^{(n)}(\xi)}{n!}$$

for some point ξ in the interval containing I and x.

We need to apply this to a polynomial of degree $n - 1 = 1$, so we obtain

$$f(x) - p_1(x) = \frac{(x - x_i)(x - x_{i+1}) f''(\xi)}{2}$$

Unquiz: Suppose that the absolute value of the second derivative of f is bounded by 25. How many equally-spaced knots do we need to guarantee that the difference between f and the interpolant is less than $.001$?

Adaptive interpolation

If we have a choice, it may be better to use non-equal spacing of the knots.

See p. 111.

Cubic interpolation

Cubic interpolation

- ordinary cubic polynomials: 3 continuous nonzero derivatives.
- cubic splines: 2 continuous nonzero derivatives.
- Hermite cubics: 1 continuous nonzero derivative.

Cubic splines and Hermite cubics are the most commonly used piecewise-polynomial interpolants.

We'll just study cubic splines, but Section 3.2 is good if you want to learn about Hermite cubics.

Cubic Splines

Splines

A function $s(x)$ is a spline of degree k with knots $a = x_1 < \ldots < x_n = b$ if

1. in every interval $[x_i, x_{i+1}]$, s is a polynomial of degree $\leq k$.
2. s, s', ..., $s^{(k-1)}$ are continuous functions.

Thus a spline is a kind of piecewise polynomial.

The most useful splines are the cubic splines: $s \in \mathcal{C}^2[a, b]$ and s is a polynomial of degree 3 or less in each interval.

We use splines to interpolate data $s(x_i) = f_i$.

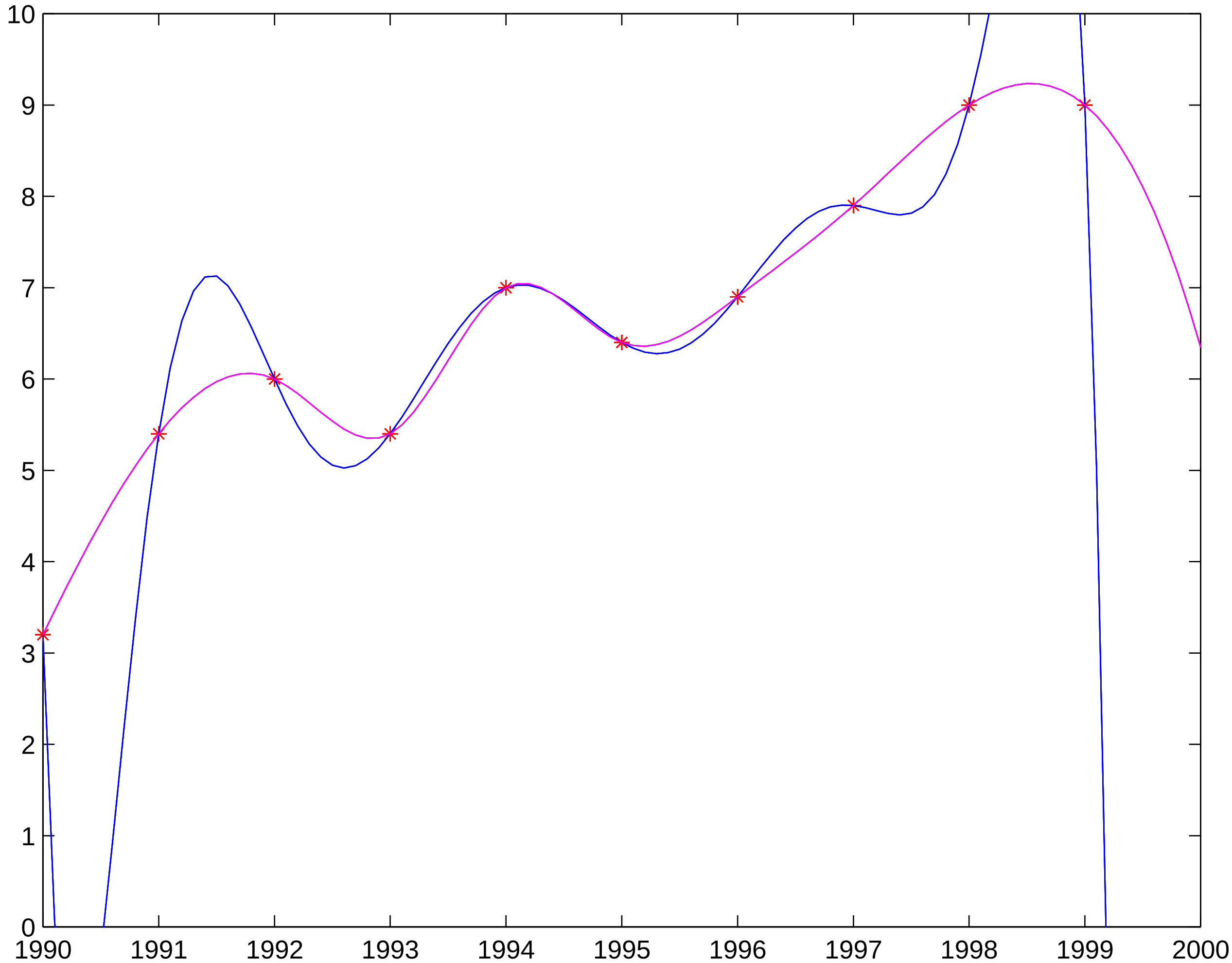

Figure 1: Matlab's default spline fit to our pollution data, compared with the polynomial fit

Pollution, revisited

Questions about spline interpolation

- existence
- uniqueness
- good basis for computation
- convergence

One good basis

Notation:

- $h_{i+1} = x_{i+1} - x_i$, $i = 1, \ldots, n-1$
- $k_{i+1} = f_{i+1} - f_i$, $i = 1, \ldots, n-1$
- $I_{i+1} = [x_i, x_{i+1}]$, $i = 1, \ldots, n-1$

We will set $s(x)$ equal to $s_{i+1}(x)$ on interval I_{i+1}, where

$$s_{i+1}(x) = m_i \frac{(x_{i+1} - x)^3}{6h_{i+1}} + m_{i+1} \frac{(x - x_i)^3}{6h_{i+1}} + a_i(x - x_i) + b_i$$

for some constants m_i, m_{i+1}, a_i, and b_i.

Note: This is slightly different from Van Loan's choice, but yields a very similar system of equations.

Now we impose the conditions on the spline in order to determine the constants.

Interpolation conditions

$$s_{i+1}(x) = m_i \frac{(x_{i+1} - x)^3}{6h_{i+1}} + m_{i+1} \frac{(x - x_i)^3}{6h_{i+1}} + a_i(x - x_i) + b_i$$

1. For $i = 1, \ldots, n-1$,

$$s_{i+1}(x_i) = f_i = m_i \frac{h_{i+1}^3}{6h_{i+1}} + m_{i+1}0 + a_i 0 + b_i \,.$$

Therefore,

$$b_i = f_i - m_i \frac{h_{i+1}^2}{6} \,.$$

$$s_{i+1}(x) = m_i \frac{(x_{i+1}-x)^3}{6h_{i+1}} + m_{i+1} \frac{(x-x_i)^3}{6h_{i+1}} + a_i(x-x_i) + b_i$$

2. For $i = 1, \ldots, n-1$,

$$s_{i+1}(x_{i+1}) = f_{i+1} = m_i 0 + m_{i+1} \frac{h_{i+1}^3}{6h_{i+1}} + a_i h_{i+1} + b_i \,.$$

Therefore,

$$a_i = \frac{f_{i+1} - b_i - m_{i+1}\frac{h_{i+1}^2}{6}}{h_{i+1}} \,,$$

so

$$a_i = \frac{f_{i+1} - f_i}{h_{i+1}} - \frac{h_{i+1}}{6}(m_{i+1} - m_i)$$

So we have formulas for all of the as and bs in terms of the ms, and we have ensured that s is continuous.

Continuity of s'

$$s_{i+1}(x) = m_i \frac{(x_{i+1}-x)^3}{6h_{i+1}} + m_{i+1} \frac{(x-x_i)^3}{6h_{i+1}} + a_i(x-x_i) + b_i$$

3. For $i = 1, \ldots, n-1$,

$$s'_{i+1}(x) = -\frac{m_i}{2h_{i+1}}(x_{i+1}-x)^2 + \frac{m_{i+1}}{2h_{i+1}}(x-x_i)^2 + a_i \,.$$

Therefore, $s'_{i+1}(x_i) = s'_i(x_i)$ if

$$-\frac{m_i}{2h_{i+1}} h_{i+1}^2 + a_i = \frac{m_i}{2h_i} h_i^2 + a_{i-1} \,, i = 2, \ldots, n-1.$$

Since $a_i = \frac{k_{i+1}}{h_{i+1}} - \frac{h_{i+1}}{6}(m_{i+1} - m_i)$, we have

$$-\frac{m_i}{2} h_{i+1} + \frac{k_{i+1}}{h_{i+1}} - \frac{h_{i+1}}{6}(m_{i+1} - m_i) = \frac{m_i}{2} h_i + \frac{k_i}{h_i} - \frac{h_i}{6}(m_i - m_{i-1}) \,.$$

Finally, continuity of s''

$$s'_{i+1}(x) = -\frac{m_i}{2h_{i+1}}(x_{i+1}-x)^2 + \frac{m_{i+1}}{2h_{i+1}}(x-x_i)^2 + a_i\,.$$

4. For $i = 1, \ldots, n-1$,

$$s''_{i+1}(x) = +\frac{m_i}{h_{i+1}}(x_{i+1}-x) + \frac{m_{i+1}}{h_{i+1}}(x-x_i)\,.$$

Therefore, $s''_{i+1}(x_i) = m_i = s''_i(x_i)$ for $i = 2, \ldots, n-1$, so continuity of this derivative is built into the representation!

Note that

$$\begin{aligned} s''(x_1) &= s_1(x_1) = m_1 \\ s''(x_n) &= s_n(x_n) = m_n \end{aligned}$$

Summary

Our function s is an interpolating cubic spline if, for $i = 2, \ldots, n-1$,

$$-\frac{m_i}{2}h_{i+1} + \frac{k_{i+1}}{h_{i+1}} - \frac{h_{i+1}}{6}(m_{i+1}-m_i) = \frac{m_i}{2}h_i + \frac{k_i}{h_i} - \frac{h_i}{6}(m_i - m_{i-1})\,.$$

and thus the parameters m_i, which are second derivatives at the knots, can be determined from the linear equations

$$\frac{h_i}{6}m_{i-1} + \frac{h_{i+1}+h_i}{3}m_i + \frac{h_{i+1}}{6}m_{i+1} = -\frac{k_i}{h_i} + \frac{k_{i+1}}{h_{i+1}} \equiv -\gamma_i + \gamma_{i+1}\,.$$

If we set $c_i = h_i/6$, then we can write the system as

$$\begin{bmatrix} c_2 & 2(c_2+c_3) & c_3 & & & & \\ & c_3 & 2(c_3+c_4) & c_4 & & & \\ & \cdot & \cdot & \cdot & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & c_{n-1} & 2(c_{n-1}+c_n) & c_n \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ \cdot \\ \cdot \\ \cdot \\ m_n \end{bmatrix} = \begin{bmatrix} -\gamma_2+\gamma_3 \\ -\gamma_3+\gamma_4 \\ \cdot \\ \cdot \\ \cdot \\ -\gamma_{n-1}+\gamma_n \end{bmatrix}$$

Notes:

- This is a set of $n-2$ equations in n unknowns.
- The rows of the matrix are linearly independent. (Prove this by finite induction: the kth is independent of the first $k-1$.)
- Therefore, the solution exists, but is not unique. We need two more conditions to impose uniqueness.

Common choices of end conditions

- The natural cubic spline interpolant: $s''(a) = s''(b) = 0$
- The periodic cubic spline interpolant: $s^{(k)}(a) = s^{(k)}(b)$, $k = 0, 1, 2$.
- The complete cubic spline interpolant: $s'(a)$ and $s'(b)$ given.
- The not-a-knot cubic spline interpolant: make the third derivative of s continuous at x_2 and x_{n-1} so that these points are not knots.

The natural cubic spline interpolant

$$\begin{bmatrix} 2(c_2+c_3) & c_3 & & & \\ c_3 & 2(c_3+c_4) & c_4 & & \\ \cdot & \cdot & \cdot & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & & c_{n-1} & 2(c_{n-1}+c_n) \end{bmatrix} \begin{bmatrix} m_2 \\ m_3 \\ \cdot \\ \cdot \\ \cdot \\ m_{n-1} \end{bmatrix} = \begin{bmatrix} -\gamma_2+\gamma_3 \\ -\gamma_3+\gamma_4 \\ \cdot \\ \cdot \\ \cdot \\ -\gamma_{n-1}+\gamma_n \end{bmatrix}$$

We prove that the matrix (call it A) is nonsingular by contradiction. Suppose there is a nonzero vector z such that $Az = 0$. Suppose that z_k is its maximum magnitude component, and, without loss of generality, z_k is positive.

Then

$$2(c_k + c_{k+1})z_k + c_k z_{k-1} + c_{k+1} z_{k+1} = 0$$

(although one of the two last terms may be absent). Therefore,

$$c_k(2z_k + z_{k-1}) + c_{k+1}(2z_k + z_{k+1}) = 0.$$

But c_k, c_{k+1}, and the quantities in parentheses are positive, so this is a contradiction, unless $z = 0$.

Therefore, A is nonsingular and the solution exists and is unique.

The complete spline

Unquiz: Write the equations and prove existence and uniqueness of the solution.

The software

Matlab's `spline` function computes the not-a-knot spline.

```
z = [0:.1:6];   % points for evaluation
x = [1 2 -1 0];
y = [3 5 4 6];
Svals = spline(x,y,z);
plot(z,Svals)
```

or

```
S = spline(x,y);
Svals = ppval(S,z);
```

Summary:

We have shown

- existence,
- uniqueness,
- and computability

for the interpolating cubic spline.

Next we need to establish some approximability and convergence properties.

The minimization property of cubic splines

Some background:

- Function space $\mathcal{L}^2[a,b]$ is the set of functions $f : [a,b] \to \mathcal{R}$ such that

$$\|f\|^2 = \int_a^b |f(t)|^2 dt < \infty .$$

- A function $f : [a,b] \to \mathcal{R}$ is absolutely continuous if for every $\epsilon > 0$ there exists a $\delta > 0$ such that

$$\sum_i |f(b_i) - f(a_i)| < \epsilon$$

  for every finite set of points $a \le a_1 < b_1 < \ldots < a_n < b_n \le b$ satisfying $\sum_i |b_i - a_i| < \delta$. (Lipschitz continuous functions are absolutely continuous.)

  If a function is absolutely continuous, then it is continuous and f' exists almost everywhere.

- Function space $\mathcal{K}^2[a,b]$ is the set of functions $f : [a,b] \to \mathcal{R}$ such that f' is absolutely continuous on $[a,b]$ and $f'' \in \mathcal{L}^2[a,b]$.

Minimum Norm property of splines

Theorem: Given (x_i, f_i), $i = 1, \ldots, n$, let $\hat{s}$ be the spline that interpolates this data (using any of our choices of extra conditions). Then, for all $f \in \mathcal{K}^2[a,b]$ that match this data and extra conditions,

$$\|f - \hat{s}\|^2 = \|f\|^2 - \|\hat{s}\|^2 \ge 0 .$$

Implication: The spline is the minimum energy function that interpolates the data.

Convergence properties of complete splines

Theorem: Let $f \in \mathcal{C}^4[a,b]$, and let $|f^{(4)}(x)| \le L$ for some given number L and all $x \in [a,b]$. Let s be the complete interpolating spline with knots $x_1, \ldots, x_n$, and choose $K = \|\delta\|_\infty / \min h_i$. Then there exist constants $C_k \le 2$, independent of the knots, such that

$$|f^{(k)}(x) - s^{(k)}(x)| \le C_k L K \|\delta\|_\infty^{4-k}$$

for $k = 0, 1, 2, 3$.

Conclusions

- Splines give good approximations to functions and derivatives. The minimum energy property means that they tend to have fewer "bends" than polynomials and other interpolants.

- Given a sequence of meshes δ_1, $\delta_2, \ldots$, with

$$\frac{\delta_m}{|x_{j+1}^m - x_j^m|} \le K < \infty \,,$$

the spline approximation will converge.

Physical splines

Cubic splines are a mathematical model of physical splines, which minimize the curvature $f''(x)(1 + (f'(x))^2)^{-3/2}$.

Final Words

- Spline interpolation is much more practical for data fitting than polynomial interpolation.