7. Interpolation

- polynomial interpolation
- Newton divided difference
- Lagrange interpolation
- spline interpolation

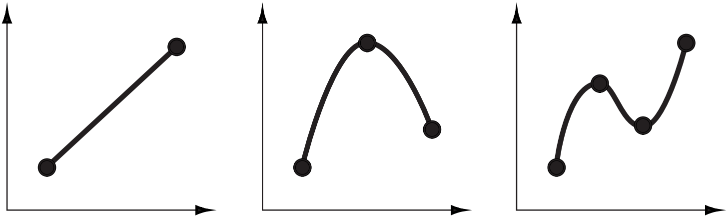
Polynomial interpolation

construct an nth-order polynomial

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

that passes exactly through the given data points

- for $n + 1$ data points $\Rightarrow$ unique nth order polynomial
- examples: (a) $n = 1$ straight line; (b) $n = 2$ parabola; (c) $n = 3$



(a) (b) (c)

Why polynomial interpolation?

- simple conceptual framework
- used for prediction: provides a formula to estimate *intermediate values* directly
- building blocks for other, more complex algorithms in differentiation, integration, solution of differential equations, approximation theory, ...
- *e.g.*, finding approximations for derivatives and integrals of a complicated function

Interpolating polynomial via linear systems

fit polynomial $f(x) = \sum_{k=0}^{n} a_k x^k$ to data $(x_0, f(x_0)), \ldots, (x_n, f(x_n))$

- substitute values $\{(x_i, f(x_i))\}_{i=0}^{n}$ in $f(x)$ yields $n+1$ linear equations:

$$\begin{bmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix}$$

  coefficient matrix called *Vandermonde matrix*

- given three points $(x_0, f(x_0)),\ (x_1, f(x_1)),\ (x_2, f(x_2))$, substitute to obtain

$$\begin{aligned} f(x_0) &= a_0 + a_1 x_0 + a_2 x_0^2 \\ f(x_1) &= a_0 + a_1 x_1 + a_2 x_1^2 \\ f(x_2) &= a_0 + a_1 x_2 + a_2 x_2^2 \end{aligned} \quad \Longrightarrow \quad \begin{bmatrix} 1 & x_0 & x_0^2 \\ 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ f(x_2) \end{bmatrix}$$

Efficiency and numerical cautions

Solving Vandemonde system

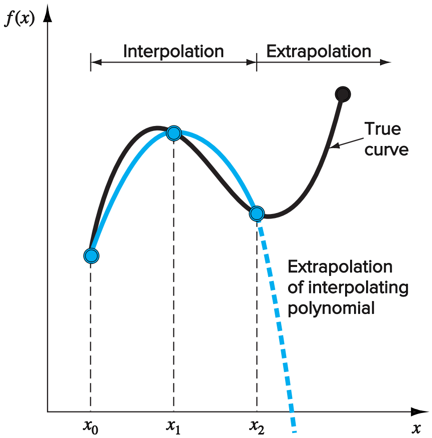
- forming and solving a full Vandermonde system is not the most efficient path
- Vandermonde matrices are ill-conditioned for large n or widely spaced x_i
- small data or rounding errors can produce large coefficient errors

Special algorithms

- specialized algorithms are faster and more stable
- two forms especially useful for computer implementation:
  1. *Newton polynomial*
  2. *Lagrange polynomial*
- allows forming $f(x)$ directly without solving for all a_k

Extrapolation

- *interpolation:* x is inside the smallest interval containing all the data
- *extrapolation:* x is outside that interval



Outline

- polynomial interpolation
- **Newton divided difference**
- Lagrange interpolation
- spline interpolation

Linear interpolation (first-order)

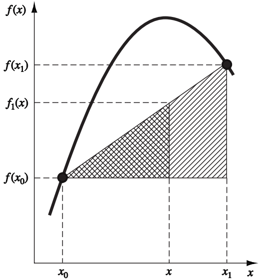
- connect two data points $(x_0, f(x_0))$ and $(x_1, f(x_1))$ with a straight line

- from similar triangles, we get the **linear interpolation formula**

$$\frac{f_1(x) - f(x_0)}{x - x_0} = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

$$\Longrightarrow$$

$$f_1(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0)$$



- slope $f[x_1, x_0] = \frac{f(x_1)-f(x_0)}{x_1-x_0}$ is first *finite divided difference* of 1st-derivative
  - as $x_1 \to x_0$, first divided difference $f[x_1, x_0] \to f'(x_0)$ for smooth f

- as interval $[x_0, x_1]$ shrinks, f is better approximated by a straight line

Example

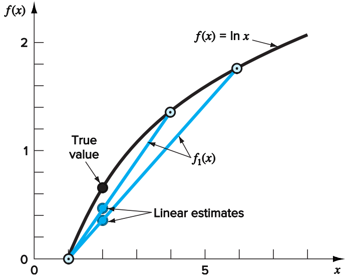
estimate $\ln 2 = 0.6931472$ on $[1, 6]$ and $[1, 4]$

(a) interpolate on $[1, 6]$: using $\ln 1 = 0, \ln 6 = 1.791759$,

$$f_1(2) = 0 + \frac{1.791759 - 0}{6-1}(2-1) = 0.3583519, \quad \varepsilon_t = 48.3\%$$

(b) interpolate on $[1, 4]$: using $\ln 1 = 0, \ln 4 = 1.386294$,

$$f_1(2) = 0 + \frac{1.386294 - 0}{4-1}(2-1) = 0.4620981, \quad \varepsilon_t = 33.3\%$$



Quadratic (parabola) interpolation (second-order)

to introduce *curvature*, use three points $(x_0, f(x_0))$, $(x_1, f(x_1))$, $(x_2, f(x_2))$

Newton form quadratic polynomial

$$f_2(x) = b_0 + b_1(x - x_0) + b_2(x - x_0)(x - x_1)$$

- equivalent to the standard quadratic $a_0 + a_1 x + a_2 x^2$ via collecting terms
- coefficients determined by enforcing exactness at x_0, x_1, x_2:

$$b_0 = f(x_0), \quad b_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

$$b_2 = \frac{\dfrac{f(x_2) - f(x_1)}{x_2 - x_1} - \dfrac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0}$$

- b_1 is *first divided difference*, and b_2 is *second divided difference*

Example

use quadratic interpolation for $\ln 2$ given data

$$x_0 = 1,\ f(x_0) = 0; \quad x_1 = 4,\ f(x_1) = 1.386294; \quad x_2 = 6,\ f(x_2) = 1.791759$$

using previous formulas, we have

$$b_0 = f(x_0) = 0, \quad b_1 = \frac{1.386294 - 0}{4 - 1} = 0.4620981,$$

$$b_2 = \frac{\dfrac{1.791759 - 1.386294}{6 - 4} - 0.4620981}{6 - 1} = -0.0518731$$

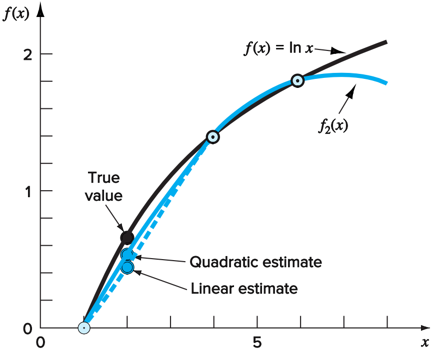
hence, the interpolant:

$$f_2(x) = 0 + 0.4620981(x - 1) - 0.0518731(x - 1)(x - 4)$$

and the estimated value at $x = 2$ is

$$f_2(2) = 0.5658444, \qquad \varepsilon_t = \frac{0.6931472 - 0.5658444}{0.6931472} \times 100\% = 18.4\%$$

Example



- quadratic interpolant improves over linear case; added curvature reduces error
- linear: exact at x_0, x_1; error proportional to local curvature (second derivative)
- quadratic: exact at x_0, x_1, x_2; incorporates a second-order term via b_2, thus better tracks smooth curvature of $\ln x$ near $x = 2$

Newton's interpolating polynomial

general nth-order interpolating polynomial for $n+1$ points:

$$f_n(x) = b_0 + b_1(x-x_0) + b_2(x-x_0)(x-x_1) + \cdots + b_n(x-x_0)(x-x_1)\cdots(x-x_{n-1})$$

- coefficients b_j are determined by **finite divided differences**:

$$b_0 = f(x_0),\ b_1 = f[x_1, x_0],\ b_2 = f[x_2, x_1, x_0],\ \ldots,\ b_n = f[x_n, x_{n-1}, \ldots, x_0]$$

- recursive definitions:

$$f[x_i, x_j] = \frac{f(x_i) - f(x_j)}{x_i - x_j}$$ 1st finite divided difference

$$\vdots$$

$$f[x_i, x_j, x_k] = \frac{f[x_i, x_j] - f[x_j, x_k]}{x_i - x_k}$$ 2nd finite divided difference

$$\vdots$$

$$f[x_n, \ldots, x_0] = \frac{f[x_n, \ldots, x_1] - f[x_{n-1}, \ldots, x_0]}{x_n - x_0}$$ nth finite divided difference

Recursive computation of divided differences

- example structure:

i	x_i	$f(x_i)$	First	Second	Third
0	x_0	$f(x_0)$	$f[x_1, x_0]$	$f[x_2, x_1, x_0]$	$f[x_3, x_2, x_1, x_0]$
1	x_1	$f(x_1)$	$f[x_2, x_1]$	$f[x_3, x_2, x_1]$	
2	x_2	$f(x_2)$	$f[x_3, x_2]$		
3	x_3	$f(x_3)$			

- the divided difference coefficients satisfy the recursive formula

$$f[x_i, x_{i-1}, \ldots, x_0] = \frac{f[x_i, \ldots, x_1] - f[x_{i-1}, \ldots, x_0]}{x_i - x_0}$$

  require to compute for $0 \le k < j \le i \le n$:

$$f[x_j] = f(x_j), \quad f[x_j, \ldots, x_k] = \frac{f[x_j, \ldots, x_{k+1}] - f[x_{j-1}, \ldots, x_k]}{x_j - x_k}$$

- higher-order differences are computed from lower-order ones

- this recursive property is the basis of efficient computer algorithms

Example

extend last example to cubic interpolation for $\ln 2$ using points

$$x_0 = 1,\ f(x_0) = 0; \quad x_1 = 4,\ f(x_1) = 1.386294$$
$$x_2 = 6,\ f(x_2) = 1.791759; \quad x_3 = 5,\ f(x_3) = 1.609438$$

i	x_i	$f[x_i]$	$f[x_{i+1}, x_i]$	$f[x_{i+2}, x_{i+1}, x_i]$	$f[x_3, x_2, x_1, x_0]$
0	1	0	0.4620981	-0.05187311	0.007865529
1	4	1.386294	0.2027326	-0.02041100	
2	6	1.791759	0.1823216		
3	5	1.609438			

for example

$$f[x_1, x_0] = \frac{1.386294 - 0}{4 - 1} = 0.4620981$$
$$f[x_2, x_1, x_0] = \frac{0.2027326 - 0.4620981}{6 - 1} = -0.05187311$$
$$f[x_3, x_2, x_1, x_0] = \frac{-0.02041100 - (-0.05187311)}{5 - 1} = 0.007865529$$

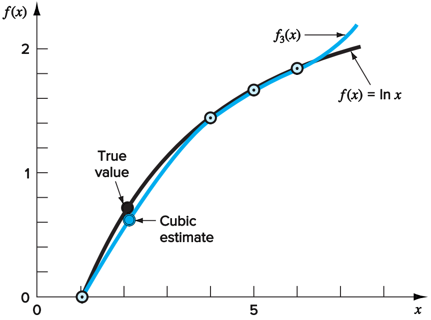
Example

resulting polynomial coefficient from first row:

$$f_3(x) = 0 + 0.4620981(x-1) - 0.05187311(x-1)(x-4)$$
$$+ 0.007865529(x-1)(x-4)(x-6)$$

estimate at $x = 2$ (true value $\ln 2 = 0.6931472$):

$$f_3(2) = 0.6287686, \quad \varepsilon_t = \frac{0.6931472 - 0.6287686}{0.6931472} \times 100\% = 9.3\%$$



Errors of Newton's interpolating polynomials

- structure of Newton's polynomial resembles a Taylor series expansion

$$f_n(x) = f(x_0) + (x - x_0) f[x_1, x_0] + \cdots$$

- if $f(x)$ is truly an nth-order polynomial, the interpolating polynomial is exact
- analogy with Taylor series remainder for nth order polynomial:

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)(x - x_1)\cdots(x - x_n), \quad \xi \text{ lies within the data interval}$$

- practical difficulty: $f^{(n+1)}(\xi)$ is usually unknown
- alternative finite difference formulation

$$R_n = f[x, x_n, \ldots, x_0](x - x_0)(x - x_1)\cdots(x - x_n)$$

- if an extra data point $f(x_{n+1})$ is available, error can be estimated as

$$R_n \approx f[x_{n+1}, x_n, \ldots, x_0](x - x_0)(x - x_1)\cdots(x - x_n) = f_{n+1}(x) - f_n(x)$$

Example: error estimation

estimate error of quadratic case for $\ln 2$ using an extra data point $f(5) = 1.609438$

- quadratic estimate $f_2(2) = 0.5658444$
- true error

$$E_t = 0.6931472 - 0.5658444 = 0.1273028$$

- error estimate:

$$\begin{aligned} R_2 &= f[x_3, x_2, x_1, x_0](x-1)(x-4)(x-6) \\ &= 0.007865529(2-1)(2-4)(2-6) = 0.0629242 \end{aligned}$$

estimate is of the same order of magnitude as the true error

Outline

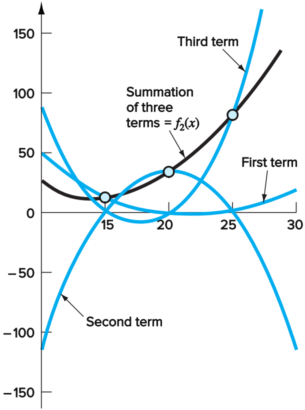
- polynomial interpolation
- Newton divided difference
- **Lagrange interpolation**
- spline interpolation

Lagrange interpolating polynomials

$$f_n(x) = \sum_{i=0}^{n} L_i(x) f(x_i)$$

where

$$L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$



- a reformulation of Newton's polynomial that avoids divided differences
- each $L_i(x)$ is 1 at $x = x_i$ and 0 at other sample points
- the sum is the unique nth-order polynomial that passes through all $n + 1$ points

First-, second-, third-order Lagrange polynomial

- first-order polynomial ($n = 1$):

$$f_1(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

- second-order polynomial ($n = 2$):

$$\begin{aligned} f_2(x) = {} & \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) \\ & + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2) \end{aligned}$$

- third-order polynomial ($n = 3$):

$$\begin{aligned} f_3(x) = {} & \frac{(x - x_1)(x - x_2)(x - x_3)}{(x_0 - x_1)(x_0 - x_2)(x_0 - x_3)} f(x_0) + \frac{(x - x_0)(x - x_2)(x - x_3)}{(x_1 - x_0)(x_1 - x_2)(x_1 - x_3)} f(x_1) \\ & + \frac{(x - x_0)(x - x_1)(x - x_3)}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3)} f(x_2) + \frac{(x - x_0)(x - x_1)(x - x_2)}{(x_3 - x_0)(x_3 - x_1)(x_3 - x_2)} f(x_3) \end{aligned}$$

Example

use Lagrange first-order interpolation to estimate $\ln 2$ with data

$$x_0 = 1,\ f(x_0) = 0,\ x_1 = 4,\ f(x_1) = 1.386294$$

we have

$$f_1(2) = \frac{2-4}{1-4} \cdot 0 + \frac{2-1}{4-1} \cdot 1.386294 = 0.4620981$$

extending the example with three points

$$x_0 = 1,\ f(x_0) = 0,\ x_1 = 4,\ f(x_1) = 1.386294,\ x_2 = 6,\ f(x_2) = 1.791760$$

gives

$$\begin{aligned} f_2(2) &= \frac{(2-4)(2-6)}{(1-4)(1-6)} \cdot 0 + \frac{(2-1)(2-6)}{(4-1)(4-6)} \cdot 1.386294 \\ &+ \frac{(2-1)(2-4)}{(6-1)(6-4)} \cdot 1.791760 = 0.5658444 \end{aligned}$$

Observation: agrees with the Newton interpolation

Example: parachutist velocity interpolation problem

estimate $v(10)$ by polynomial interpolation of orders $n = 1, 2, 3, 4$ given data

t	1	3	5	7	13
v	800	2310	3090	3940	4755

(a) quartic ($n = 4$): use all five points

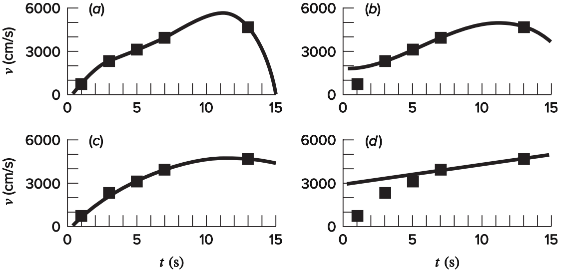
(b) cubic ($n = 3$): use $\{(3, 2310), (5, 3090), (7, 3940), (13, 4755)\}$

(c) quadratic ($n = 2$): use $\{(5, 3090), (7, 3940), (13, 4755)\}$

(d) linear ($n = 1$): use $\{(7, 3940), (13, 4755)\}$

note: selecting nearest neighbors typically improves stability and accuracy

Computed estimates at $t = 10$ s



- higher orders (cubic, quartic) *overshoot* trend between $t = 7$ and $t = 13$
- higher-degree polynomials are ill-conditioned and sensitive to data spacing/noise
- prefer *low-order* interpolation with *nearby* points for local estimates
- for noisy data, consider *regression* (least squares) rather than exact interpolation
- for many points over a range, consider *piecewise* low-order methods (*e.g.*, splines)

Inverse interpolation

- inverse problem: given $f(x)$, determine x
- *e.g.*, find x such that $f(x) = \frac{1}{x} = 0.3 \Rightarrow$ true value $x = 3.333$
- x values typically evenly spaced
- example: $f(x) = 1/x$

x	1	2	3	4	5	6	7
$f(x)$	1	0.5	0.3333	0.25	0.2	0.1667	0.1429

Naive approach: swap variables and interpolate x vs $f(x)$

$y = f(x)$	0.1429	0.1667	0.2	0.25	0.3333	0.5	1
$g(y) = x$	7	6	5	4	3	2	1

- but $f(x)$ values are nonuniform $\Rightarrow$ abscissa “telescoped”
- this often causes oscillations even with low-order polynomials

Polynomial strategy for inverse interpolation

alternative approach:

- fit interpolating polynomial $f_n(x)$ to original data ($f(x)$ vs x)
- then solve $f_n(x) = f^*$ for x using root-finding

Example: fit quadratic through $(2, 0.5), (3, 0.3333), (4, 0.25)$

$$f_2(x) = 1.08333 - 0.375x + 0.041667x^2$$

solve for $f(x) = 0.3$:

$$0.3 = 1.08333 - 0.375x + 0.041667x^2$$

quadratic formula:

$$x = \frac{0.375 \pm \sqrt{(-0.375)^2 - 4(0.041667)(0.78333)}}{2(0.041667)}$$

roots: $x = 5.704,\ 3.296$

$\Rightarrow$ choose $x = 3.296$ as approximation to true 3.333

Outline

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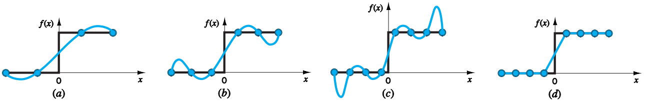
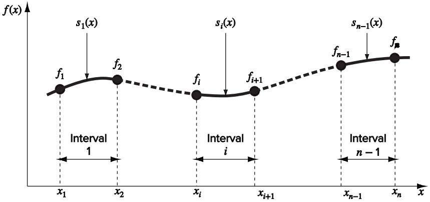
- Newton divided difference
- Lagrange interpolation
- **spline interpolation**

Spline interpolation

- apply lower-order polynomials to subsets of data points
- these connecting polynomials are called **spline functions**



- higher-order polynomials oscillate wildly near abrupt changes
- splines (limited to lower-order curves) minimize oscillations
- for n data points, there are $n-1$ intervals; each interval i has spline $s_i(x)$



data points where two splines meet are called *knots* or *break points*

Linear splines

straight line between two adjacent points with $[x_i, x_{i+1}]$, $i = 1, \dots, n-1$

Linear spline: for interval $[x_i, x_{i+1}]$, use Newton's first-order polynomial

$$s_i(x) = a_i + b_i(x - x_i), \qquad a_i = f_i, \quad b_i = \frac{f_{i+1} - f_i}{x_{i+1} - x_i}$$

therefore,

$$s_i(x) = f_i + \frac{f_{i+1} - f_i}{x_{i+1} - x_i}(x - x_i), \quad \text{for} \quad x \in [x_i, x_{i+1}]$$

- n data points $\Rightarrow$ $n - 1$ intervals
- each $s_i(x)$ can be used to evaluate f between (x_i, x_{i+1})

Example

fit the data in table with first-order splines and evaluate the function at $x = 5$

i	x_i	f_i
1	3.0	2.5
2	4.5	1.0
3	7.0	2.5
4	9.0	0.5

- 4 data points $\Rightarrow$ 3 intervals
- spline in interval i:

$$s_i(x) = f_i + \frac{f_{i+1} - f_i}{x_{i+1} - x_i}(x - x_i)$$

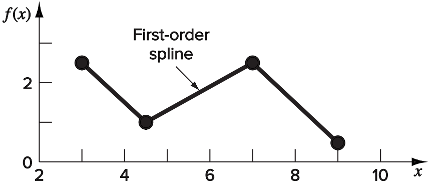
- for the second interval ($x = 4.5$ to $x = 7$),

$$s_2(x) = 1.0 + \tfrac{2.5-1.0}{7.0-4.5}(x - 4.5)$$

evaluating at $x = 5$:

$$s_2(5) = 1.0 + \tfrac{2.5-1.0}{7.0-4.5}(5 - 4.5) = 1.3$$

Example



(a)

Remarks

- first-order splines connect data with straight lines
- disadvantage: not smooth at knots (slope changes abruptly)
- first derivative is discontinuous at joining points
- higher-order splines overcome this by enforcing derivative continuity

Quadratic splines

spline of at least $n+1$ order need to ensure nth derivatives are continuous at knots

- quadratic splines require continuous first derivatives at knots
- goal: for n data points (x_i, f_i), construct piecewise quadratics on $n-1$ intervals

$$[x_i, x_{i+1}]$$

Quadratic spline: for interval i:

$$s_i(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2$$

for n data points ($i = 1, \dots, n$):

- $n-1$ intervals $\Rightarrow$ $3(n-1)$ unknowns (a_i, b_i, c_i)
- need $3(n-1)$ conditions to solve system

Conditions for quadratic splines

Continuity at points (pass through data)

$$f_i = a_i + b_i(x_i - x_i) + c_i(x_i - x_i)^2 \quad \Rightarrow \quad a_i = f_i$$

so

$$s_i(x) = f_i + b_i(x - x_i) + c_i(x - x_i)^2$$

reduces unknowns to $2(n-1)$

Function continuity at knots: define $h_i = x_{i+1} - x_i$, then

$$s_i(x_{i+1}) = s_{i+1}(x_{i+1}) \Longrightarrow f_i + b_i h_i + c_i h_i^2 = f_{i+1}$$

Derivative continuity at interior knots

$$s_i'(x) = b_i + 2c_i(x - x_i) \Longrightarrow b_i + 2c_i h_i = b_{i+1}$$

Zero second derivative at first point

$$c_1 = 0$$

this implies first two points will be connected by a straight line

Example

fit quadratic splines to the data

i	x_i	f_i
1	3.0	2.5
2	4.5	1.0
3	7.0	2.5
4	9.0	0.5

use the results to estimate the value of the function at $x = 5$

- for four data points ($n = 4$) we have $n - 1 = 3$ intervals
- after continuity condition and zero 2nd-derivative condition ($c_1 = 0$), we need

$$2(4-1) - 1 = 5$$

  conditions

Example

continuity at knots yields (with $c_1 = 0$)

$$
\begin{aligned}
f_1 + b_1 h_1 &= f_2 \\
f_2 + b_2 h_2 + c_2 h_2^2 &= f_3 \\
f_3 + b_3 h_3 + c_3 h_3^2 &= f_4
\end{aligned}
$$

derivative continuity conditions (with $c_1 = 0$)

$$
\begin{aligned}
b_1 &= b_2 \\
b_2 + 2c_2 h_2 &= b_3
\end{aligned}
$$

function and interval widths $h_1 = 1.5,\ h_2 = 2.5,\ h_3 = 2.0$

putting things together, results in the system of linear equations:

$$
\begin{bmatrix} 1.5 & 0 & 0 & 0 & 0 \\ 0 & 2.5 & 6.25 & 0 & 0 \\ 0 & 0 & 0 & 2 & 4 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & 1 & 5 & -1 & 0 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ c_2 \\ b_3 \\ c_3 \end{bmatrix} = \begin{bmatrix} -1.5 \\ 1.5 \\ -2 \\ 0 \\ 0 \end{bmatrix}
$$

Example

solution is

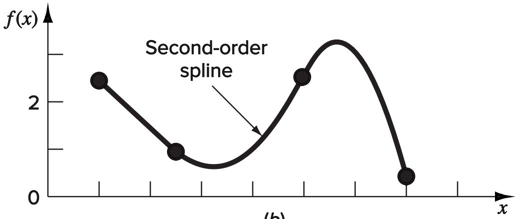
$$b_1 = -1, \quad b_2 = -1, \quad c_2 = 0.64, \quad b_3 = 2.2, \quad c_3 = -1.6$$

and the quadratic splines are

$$s_1(x) = 2.5 - (x - 3)$$
$$s_2(x) = 1.0 - (x - 4.5) + 0.64(x - 4.5)^2$$
$$s_3(x) = 2.5 + 2.2(x - 7.0) - 1.6(x - 7.0)^2$$

so, our estimate at $x = 5$ is

$$s_2(5) = 1.0 - (0.5) + 0.64(0.5^2) = 0.66$$



(b)

Cubic splines

- linear and quadratic splines lack smoothness or symmetry
- cubic splines are most commonly used
- require continuous 1st and 2nd derivatives at knots
- goal: for n data points (x_i, f_i), construct piecewise cubics on $n-1$ intervals

$$[x_i, x_{i+1}]$$

Cubic splines: for each interval on interval i, use

$$s_i(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3$$

unknowns per interval: $a_i, b_i, c_i, d_i \Rightarrow$ total $4(n-1)$ unknowns

Cubic spline interpolation

on $[x_i, x_{i+1}]$,

$$s_i(x) = f_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3$$

---

1. solve tridiagonal system for $c_1, \ldots, c_n$:

$$\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ h_1 & 2(h_1 + h_2) & h_2 & & \\ & \ddots & \ddots & \ddots & \\ & & h_{n-2} & 2(h_{n-2} + h_{n-1}) & h_{n-1} \\ 0 & \cdots & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{n-1} \\ c_n \end{bmatrix} = \begin{bmatrix} 0 \\ 3(f[x_3, x_2] - f[x_2, x_1]) \\ \vdots \\ 3(f[x_n, x_{n-1}] - f[x_{n-1}, x_{n-2}]) \\ 0 \end{bmatrix}$$

2. back-substitution for remaining coefficients

$$d_i = \frac{c_{i+1} - c_i}{3h_i}$$

$$b_i = \frac{f_{i+1} - f_i}{h_i} - \frac{h_i}{3}(2c_i + c_{i+1})$$

Derivation

Continuity at points (pass through data): at $x = x_i$,

$$f_i = a_i \quad \Rightarrow \quad a_i = f_i$$

so $s_i(x) = f_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3$

Function continuity at knots: with $h_i = x_{i+1} - x_i$

$$f_i + b_i h_i + c_i h_i^2 + d_i h_i^3 = f_{i+1}$$

First-derivative continuity

$$s_i'(x) = b_i + 2c_i(x - x_i) + 3d_i(x - x_i)^2$$

at x_{i+1},

$$b_i + 2c_i h_i + 3d_i h_i^2 = b_{i+1}$$

Second-derivative continuity

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

at x_{i+1},

$$c_i + 3d_i h_i = c_{i+1}$$

Derivation

eliminate d_i:

$$d_i = \frac{c_{i+1} - c_i}{3h_i}$$

substitute back into first two equations:

$$f_i + b_i h_i + \frac{h_i^2}{3}\,(2c_i + c_{i+1}) = f_{i+1}$$

$$b_{i+1} = b_i + h_i(c_i + c_{i+1}) \Longrightarrow b_i = b_{i-1} + h_{i-1}(c_{i-1} + c_i)$$

solve first equation for b_i and shift index:

$$b_i = \frac{f_{i+1} - f_i}{h_i} - \frac{h_i}{3}\,(2c_i + c_{i+1})$$

$$b_{i-1} = \frac{f_i - f_{i-1}}{h_{i-1}} - \frac{h_{i-1}}{3}\,(2c_{i-1} + c_i)$$

we now substitute these two equations into

$$b_i = b_{i-1} + h_{i-1}(c_{i-1} + c_i)$$

Derivation

putting things together yields a relation for c:

$$h_{i-1}c_{i-1} + 2(h_{i-1} + h_i)c_i + h_i c_{i+1} = 3\left(\frac{f_{i+1} - f_i}{h_i} - \frac{f_i - f_{i-1}}{h_{i-1}}\right)$$

or with divided differences notation $f[x_i, x_j] = \dfrac{f_i - f_j}{x_i - x_j}$,

$$h_{i-1}c_{i-1} + 2(h_{i-1} + h_i)c_i + h_i c_{i+1} = 3\big(f[x_{i+1}, x_i] - f[x_i, x_{i-1}]\big)$$

in matrix form, this yields a tridiagonal system of linear equations

Natural end conditions (straight at ends): 2nd derivatives vanish at the endpoints:

$$\begin{aligned} s_1''(x_1) &= 0 \;\Rightarrow\; c_1 = 0 \\ s_{n-1}''(x_n) &= 0 \;\Rightarrow\; c_{n-1} + 3d_{n-1}h_{n-1} = c_n = 0 \end{aligned}$$

where we introduced an extraneous parameter c_n

Example

fit cubic splines to the data

i	x_i	f_i
1	3.0	2.5
2	4.5	1.0
3	7.0	2.5
4	9.0	0.5

use the results to estimate the value of the function at $x = 5$

tridiagonal system of equations

$$\begin{bmatrix} 1 & & & \\ h_1 & 2(h_1+h_2) & h_2 & \\ & h_2 & 2(h_2+h_3) & h_3 \\ & & & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 3\big(f[x_3,x_2] - f[x_2,x_1]\big) \\ 3\big(f[x_4,x_3] - f[x_3,x_2]\big) \\ 0 \end{bmatrix}$$

data values:

$$h_1 = 4.5 - 3.0 = 1.5, \quad h_2 = 7.0 - 4.5 = 2.5, \quad h_3 = 9.0 - 7.0 = 2.0$$

Example

matrix system becomes

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 1.5 & 8 & 2.5 & 0 \\ 0 & 2.5 & 9 & 2 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 4.8 \\ -4.8 \\ 0 \end{bmatrix}$$

solution: $c_1 = 0,\ c_2 = 0.8395,\ c_3 = -0.7665,\ c_4 = 0$

compute b_i and d_i:

$$b_1 = -1.4198,\ d_1 = 0.1866$$

$$b_2 = -0.1605,\ d_2 = -0.2141$$

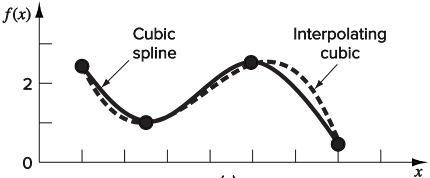
$$b_3 = 0.0221,\ d_3 = 0.1278$$

Example

final cubic splines

$$s_1(x) = 2.5 - 1.4198(x-3) + 0.1866(x-3)^3$$
$$s_2(x) = 1.0 - 0.1605(x-4.5) + 0.8395(x-4.5)^2 - 0.2141(x-4.5)^3$$
$$s_3(x) = 2.5 + 0.0221(x-7) - 0.7665(x-7)^2 + 0.1278(x-7)^3$$

estimate at $x = 5$ (interval 2): $s_2(5) = 1.103$



(c)

cubic spline fit shows smoother and more accurate behavior than linear/quadratic

End conditions for cubic splines

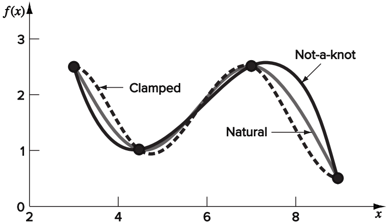
Natural condition: $c_1 = 0,\ c_n = 0$ (spline straightens at endpoints)

Clamped condition: specify first derivatives at first and last nodes

$$2h_1c_1 + h_1c_2 = 3f[x_2, x_1] - 3f'_1$$
$$h_{n-1}c_{n-1} + 2h_{n-1}c_n = 3f'_n - 3f[x_n, x_{n-1}]$$

Not-a-knot condition: enforce third derivative continuity at 2nd and next-to-last knots

$$h_2c_1 - (h_1 + h_2)c_2 + h_1c_3 = 0$$
$$h_{n-1}c_{n-2} - (h_{n-2} + h_{n-1})c_{n-1} + h_{n-2}c_n = 0$$



References and further readings

- S. C. Chapra and R. P. Canale. *Numerical Methods for Engineers* (8th edition). McGraw Hill, 2021. (Ch.18)

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