Computational Astrophysics

E. Larrañaga

Observatorio Astronómico Nacional
Universidad Nacional de Colombia

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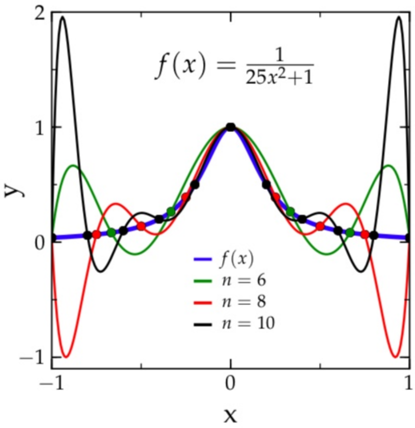
Outline

Lagrange Interpolation



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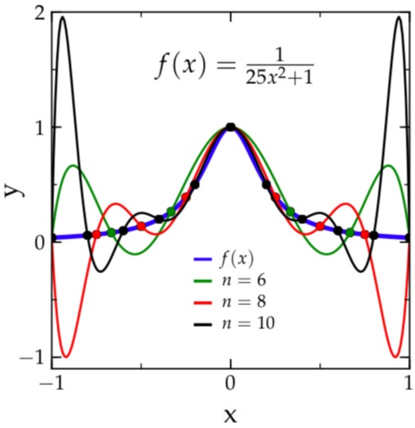
However, for most continuous functions, this is not the case ! This is called *Runge's Phenomenon*.

Lagrange Interpolation



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A higher polynomial degree could lead to a greater error and unwanted oscillations!

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The simplest form of piecewise polynomial interpolation is piecewise linear interpolation (connecting data points with straight lines).

Hermite Interpolation

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Now we will consider only the simplest case of Hermite interpolation: a function and its first derivative.
Consider $n+1$ data points. We will find a polynomial satisfying the conditions

$$p(x_i) = c_{i0}\ , \quad p'(x_i) = c_{i1} \quad \text{for } i \in [0, n]\ , \tag{2}$$

where $c_{i0} = f(x_i)$ and $c_{i1} = f'(x_i)$.

Hermite Interpolation

We propose the form

$$p(x) = \sum_{i=0}^{n} c_{i0} A_i(x) + \sum_{i=0}^{n} c_{i1} B_i(x) \ , \tag{3}$$

where $A_i(x)$ and $B_i(x)$ are polynomials satisfying:

$$\begin{aligned} A_i(x_j) &= \delta_{ij} \ , \quad & B_i(x_j) &= 0 \ , \\ A_i'(x_j) &= 0 \ , \quad & B_i'(x_j) &= \delta_{ij} \ . \end{aligned} \tag{4}$$

Hermite Interpolation

A possible form of the polynomials $A_i(x)$ and $B_i(x)$ is obtained using the Lagrange interpolation terms

$$L_{nj}(x) = \prod_{\substack{j=0 \\ k\neq j}}^{n} \frac{x - x_k}{x_j - x_k} \ , \tag{5}$$

as

$$\begin{aligned} A_i(x) &= [1 - 2(x - x_i)L'_{ni}(x_i)]L^2_{ni}(x) \ , \\ B_i(x) &= (x - x_i)L^2_{ni}(x) \ . \end{aligned} \tag{6}$$

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Each L_{ni} is of degree n and therefore A_i and B_i are of degree $2n + 1$ (The same as the maximal degree of $p(x)$).

(see proof in `http://www.math.umd.edu/~dlevy/books/na.pdf`.)

Piecewise Cubic Hermite Interpolation

Consider a dataset such that for each point x_i we also have the point x_{i+1}, as well as the values $f(x_i)$, $f(x_{i+1})$, $f'(x_i)$, and $f'(x_{i+1})$ (These values are known or can be evaluated numerically).

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Taking $n = 1$ in the Hermite interpolation equations we obtain A_i and B_i as polynomials of degree $2n + 1 = 3$.

Piecewise Cubic Hermite Interpolation

The cubic Hermite polynomial that interpolates $f(x)$ in $[x_i, x_{i+1}]$ is given by

$$\begin{aligned} H_3(x) =& f(x_i)\psi_0(z) + f(x_{i+1})\psi_0(1-z) \\ &+ f'(x_i)(x_{i+1} - x_i)\psi_1(z) \\ &- f'(x_{i+1})(x_{i+1} - x_i)\psi_1(1-z) \ , \end{aligned}$$

where

$$\psi_0(z) = 2z^3 - 3z^2 + 1 \ , \quad (7)$$

$$\psi_1(z) = z^3 - 2z^2 + z \ . \quad (8)$$

and

$$z = \frac{x - x_i}{x_{i+1} - x_i} \ , \quad (9)$$

Spline Interpolation

Splines are the ultimate method for piecewise polynomial interpolation. It achieves smoothness by requiring continuity at data points not only for the function values $f(x_i)$, but also for a number of its derivatives $f^{(\ell)}(x_i)$.

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Assuming that we know the values $f(x_i)$ at points x_i $(i \in [0, n])$, we construct piecewise polynomials of degree m on each of the n segments $[x_i, x_{i+1}]$,

$$p_i(x) = \sum_{k=0}^{m} c_{ik} x^k \ , \tag{10}$$

to approximate $f(x)$ for $x \in [x_i, x_{i+1}]$.

Spline Interpolation

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Hence, there are $n(m+1)$ coefficients c_{ik} that are determined by the conditions:

1. requiring $(n-1)(m-1)$ smoothness conditions at non-boundary points: $p_i^{\ell}(x_{i+1}) = p_{i+1}^{\ell}(x_{i+1})$ for $\ell = 1, \cdots, m-1$,
2. requiring $2n$ interpolation conditions: $p_i(x_i) = f(x_i) = p_{i+1}(x_i)$,
3. choosing the remaining $m-1$ values of some of the $p_o^{\ell}(x_o)$ and $p_{n-1}^{\ell}(x_n)$ for $\ell = 1, \cdots, m-1$.

Cubic Natural Spline Interpolation

Consider $m = 3$: Cubic Spline or *Natural* Spline.
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The first choice is to set the highest derivative to zero on both ends of the interval:

$$p_0''(x_0) = 0 \ , \ \ p_{n-1}''(x_n) = 0 \ . \tag{11}$$

Cubic Natural Spline Interpolation

Then we consider the linear interpolation of the second derivative in $[x_i, x_{i+1}]$,

$$p_i''(x) = \frac{1}{x_{i+1} - x_i}\left[(x - x_i)p_{i+1}'' - (x - x_{i+1})p_i''\right] \ , \qquad (12)$$

where $p_i'' = p_i''(x_i) = p_{i-1}''(x_i)$ and $p_{i+1}'' = p_{i+1}''(x_{i+1}) = p_i''(x_{i+1})$.

Cubic Natural Spline Interpolation

Integration of this interpolated second derivative two times and using $f_i = p_i(x_i) = f(x_i)$ gives

$$p_i(x) = \alpha_i(x - x_i)^3 + \beta_i(x - x_{i+1})^3 + \gamma_i(x - x_i) + \eta_i(x - x_{i+1}), \quad (13)$$

where

$$\alpha_i = \frac{p''_{i+1}}{6h_i} \qquad \beta_i = \frac{-p''_i}{6h_i}, \quad (14)$$

$$\gamma_i = \frac{f_{i+1}}{h_i} - \frac{h_i p''_{i+1}}{6} \qquad \eta_i = \frac{h_i p''_i}{6} - \frac{f_i}{h_i}, \quad (15)$$

with $h_i = x_{i+1} - x_i$.

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Hence, all we need to find the spline is to know all of its second derivatives $p''_i = p''_i(x_i)$.

Cubic Natural Spline Interpolation

Now apply the condition $p'_{i-1}(x_i) = p'_i(x_i)$ to the interpolated polynomial to obtain the equation

$$h_{i-1}p''_{i-1} + 2(h_{i-1} + h_i)p''_i + h_i p''_{i+1} = 6\left(\frac{g_i}{h_i} - \frac{g_{i-1}}{h_{i-1}}\right) \ , \qquad (16)$$

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where $g_i = f_{i+1} - f_i$.

This is a linear system with $n-1$ unknowns: p''_i for $i = 1, \cdots, n-1$ (remember that $p''_0 = p''_n = 0$, as set by the natural spline condition.

Cubic Natural Spline Interpolation

Defining $d_i = 2(h_{i-1} + h_i)$ and $b_i = 6\left(\frac{g_i}{h_i} - \frac{g_{i-1}}{h_{i-1}}\right)$, we can write

$$Ap'' = b \quad \text{with } A_{ij} = \begin{cases} d_i & \text{if } i = j\,, \\ h_i & \text{if } i = j-1\,, \\ h_{i-1} & \text{if } i = j+1\,, \\ 0 & \text{otherwise.} \end{cases} \tag{17}$$

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The coefficient matrix A_{ij} is real, symmetric, and tri-diagonal. The solution of such a linear system of equations will be presented later in the course.