Lecture 3: Differentiation

So far we're looked at interpolation and quadrature. In both cases, we're given data f_i at points x_i and we want to compute/estimate/approximate:

1. the function values (interpolation);
2. the definite integral (quadrature).

What about differentiation? Suppose we want to estimate the derivative of a function at a point (often, but not always, one of the x_i's).

Fit interpolating polynomial and differentiate it

This approach is conceptually simple and illustrative, although traditionally not used very often in practice (however, search for “Barycentric Lagrange”, or “Chebfun”)

Example

Suppose I want to estimate the second derivative of a function $f(x)$ at a point x_j from samples f_i and nodes x_i. How many data points do I need? Constant or linear interpolant won't work (why not?)

Simplest is quadratic.

$$f(x) = p_2(x) = f(x_0)\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + f(x_2)\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}$$

Assuming the data is equispaced, note this reduces to the gives the common “1 -2 1” rule:

$$f''(x_j) = \frac{1}{h^2}f_{j-1} - \frac{2}{h^2}f_j + \frac{1}{h^2}f_{j+1}.$$

Error analysis

What can we learn from the polynomial interpolant error formula?

Not much!

In some sense, predicts $O(h)$ which is correct when the data is not equispaced. Equispaced, it should be $O(h^2)$, which we'll see this more precisely by the next method.

Method of Undetermined Coefficients

Instead of working with interpolants, the most commonly used alternative approach is the method of undetermined coefficients.

Reference: [Chapter 1 of LeVeque 2007 Textbook].

- Based on Taylor series. Taylor expand $f(x+h)$ and $f(x-h)$ (and others) in small parameter h about x.

$$u(x+h) = u(x) + hu'(x) + \frac{h^2}{2}u''(x) + \frac{h^3}{6}u'''(x) + \frac{h^4}{24}u''''(x) + \dots$$

Examples

$$
\begin{aligned}
u(x+h) &= u(x) + hu'(x) + \frac{h^2}{2}u''(x) + \frac{h^3}{6}u'''(x) + \frac{h^4}{24}u'''''(x) + \ldots \\
&= u(x) + hu'(x) + \frac{h^2}{2}u''(x) + O(h^2)
\end{aligned}
$$

Forward difference:

$$
u'(x) = \frac{u(x+h) - u(x)}{h} + O(h)
$$

Examples

$$
\begin{aligned}
u(x-h) &= u(x) - hu'(x) + \frac{h^2}{2}u''(x) - \frac{h^3}{6}u'''(x) + \frac{h^4}{24}u'''''(x) - \dots \\
&= u(x) - hu'(x) + O(h^2)
\end{aligned}
$$

Backward difference:

$$
u'(x) = \frac{u(x) - u(x-h)}{h} + O(h)
$$

Examples

$$
\begin{aligned}
u(x+h) - u(x-h) &= 0 + 2hu'(x) + 0 - \frac{h^3}{6}u'''(x) + \dots \\
&= 2hu'(x) + O(h^3)
\end{aligned}
$$

Centered difference:

$$u'(x) = \frac{u(x+h) - u(x-h)}{2h} + O(h^2)$$

Error Analysis

- Note: this gives the $O(h^2)$ error term.
- For practical algorithms:

[Fornberg, Calculation of weights in finite difference formulas, SIAM Rev. 1998].