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, see "Barycentric Lagrange" in a later lecture, or search for "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.

[Worked example, perhaps in a CAS...]

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?

Note 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.

Example Second derivative from three data points again...

Error Analysis Note: get's the $O(h^2)$ error term.

For practical algorithms, see paper [Fornberg, Calculation of Weights in Finite Difference Formulas, SIAM Review, 1998, doi:10.1137/S0036144596322507].

Lecture 4: the Barycentric Formula

Handout: [Berrut & Trefethen, Barycentric Lagrange interpolation, SIAM Review 2004, doi:10.1137/S0036144502417715].

Consider the "Barycentric formula" for Lagrange interpolation:

$$p_n(x) = \frac{\sum_{k=0}^{n} \frac{w_k}{(x - x_k)} f_k}{\sum_{k=0}^{n} \frac{w_k}{(x - x_k)}},$$

where

$$w_k = \frac{1}{\prod_{i \neq k} (x_k - x_i)} \quad \left(= \frac{1}{w'(x_k)} \right).$$

Is this expression really the same as the Lagrange Interpolating Polynomial from Lecture 1?

What do you think could go wrong in computation?

Reference: [Higham, *The numerical stability of barycentric Lagrange interpolation*, IMAJNA 2004, doi:10.1093/imanum/24.4.547].