# 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?

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 $x$.

**Examples**   Various derivatives from three data points. Consider a smooth function $u(x)$ then

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

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

From this can show how we can compute three difference *schemes* (approximations) to $u'(x)$:

**Forward difference**:
$$u'(x) = \frac{u(x+h) - u(x)}{h} + O(h)$$

**Backward difference**:
$$u'(x) = \frac{u(x) - u(x-h)}{h} + O(h)$$

**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].

# Lecture 4: the Barycentric Formula

See: [Berrut & Trefethen, *Barycentric Lagrange interpolation*, SIAM Rev. 2004].

Consider the "Barycentric formula" for Lagrange interpolation:

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

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].