Math 5600 6/14/14

- Numerical Integration (or Quadrature)

- Obvious idea: integrate the interpolating polynomial

- $$\int_a^b \sum_{i=0}^n f(x_i) L_i(x)\,dx = \sum_{i=0}^n w_i f(x_i)$$
  $$w_i = \int_a^b L_i(x)\,dx$$ (*)

- Examples:
  $$\int_a^{a+h} f(x)\,dx \approx \frac{h\,(f(a)+f(a+h))}{2}$$

Trapezoidal (Trapezium) Rule

- Doing the same for a quadratic interpolant gives Simpson's Rule:
  $$\int_a^{a+2h} f(x)\,dx \approx \frac{h}{3}\left(f(a)+4f(a+h)+f(a+2h)\right)$$

- we could derive formulas like this using (*)

- However, there are alternatives.

- very useful concept: Method of Undetermined Coefficients.

$$\int_a^{a+2h} f(x)dx = h\left(Af(a) + Bf(a+h) + Cf(a+2h)\right)$$

$$A, B, C = ?$$

- we have a formula of a given structure, we want it to be exact for quadratic functions.
- Just look at a specific case.

e.g.: $h = 1 \quad a = -1$

$f(x) = 1, x, x^2$

$$\int_{-1}^{1} 1\,dx = 2 = A + B + C \Rightarrow B = 4/3$$

$$\left.\begin{aligned} \int_{-1}^{1} x\,dx &= 0 = -A + C \\ \int_{-1}^{1} x^2 dx &= \frac{2}{3} = A + C \end{aligned}\right\} A = C = 1/3$$

- get Simpson's Rule, again.

$$\int_a^{a+2h} f(x)dx = \frac{h}{3}\left(f(a) + 4f(a+h) + f(b)\right)$$

- What error do we expect?

- $\int_a^{a+2h} f(x)dx - \frac{h}{3}\left(f(a) + 4f(a+h) + f(a+2h)\right) = E = ?$

- Again, we expand into a Taylor series.

- All evaluations at $\underline{a+h}$ $\Leftarrow$!!

- F antiderivative of f, $F' = f$

$$E = F(a+2h) - F(a) - \frac{h}{3}\left(f(a) + 4f(a+h) + f(a+2h)\right)$$

$$= F + hF' + \frac{h^2}{2}F'' + \frac{h^3}{6}F''' + \frac{h^4}{24}F^{iv} + \frac{h^5}{120}F^{V}$$

$$-\left(F - hF' + \frac{h^2}{2}F'' - \frac{h^3}{6}F''' + \frac{h^4}{24}F^{iv} - \frac{h^5}{120}F^{V}\right)$$

$$-\frac{h}{3}\Big[\; f + hf' + \frac{h^2}{2}f'' + \frac{h^3}{6}f''' + \frac{h^4}{24}f^{IV}$$

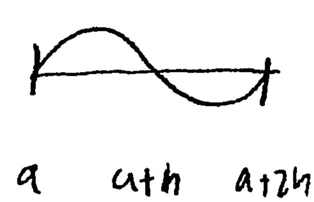
$$+ 4f$$

$$+ f - hf' + \frac{h^2}{2}f'' - \frac{h^3}{6}f''' + \frac{h^4}{24}f^{IV}\Big] + HOT$$

$$= h^5 f^{IV}\left(\frac{1}{60} - \frac{1}{36}\right) = -\frac{h^5 f^{IV}}{90} + HOT$$

- It's exact for cubics!
- How remarkable.

- Exact for



$S = 0$

- Formulas of this type are called

Newton - Cotes Formulas

- Interpolate at equally spaced points, integrate interpolating polynomial.

- Come in 2 flavors.

  - closed: include endpoints
    e.g. Trapezoidal, Simpson's

  - open: do not include endpoints,
    e.g.

$$\int_a^{a+h} f(x)\,dx \approx h f(a+\tfrac{h}{2})$$

midpoint rule.

- One could in principle use polynomials of arbitrarily high degree but just like for approximation of functions, this is not a good idea.

- Instead, it is better to apply the rules on subintervals. This gives rise to

Composite Newton-Cotes Formulas

$[a,b] \quad h = \dfrac{b-a}{N} \quad x_n = a + nh \quad n = 0, \ldots, N$

- Trapezoidal Rule

$$\int_a^b f(x)\,dx = \frac{h}{2}\left(f(a) + 2\sum_{n=1}^{N-1} f(x_i) + f(b)\right) - \frac{(b-a)h^2}{12} f''(\xi)$$

- Simpson's Rule (N is even)

$$\int_a^b f(x)\,dx = \frac{h}{3}\Big(f(a) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \cdots + 4f(x_{N-1}) + f(b)\Big) - \frac{(b-a)h^4}{90} f^{IV}(\eta)$$

- Note that we loose one power of h as we go to the composite rule.

- Notice that we multiply the function values with positive numbers.

- There is no cancellation of significant digits.

- However, as the polynomial degree goes up some of the coefficients (weights) become negative which can lead to an amplification of round-off errors

- In all cases we obtained formulas of the type

$$\int_a^b f(x)dx \approx \sum w_i f(x_i)$$

- the x_i are "knots", "nodes", or "abscissas"

- the w_i are weights.

- why should the abscissas be evenly spaced.

- We can compute the function anywhere.

- Try the method of undetermined coefficients.

- Example

$$\int_{-1}^{1} f(x)dx = w_1 f(x_1) + w_2 f(x_2)$$

- Have four parameters: w_1, x_1, w_2, x_2

- Pick them so as to have a formula that is exact for all polynomials of degree up to 3

$$f(x) = 1 \qquad \int_{-1}^{1} 1dx = 2 = w_1 + w_2$$

$$f(x) = x \qquad \int_{-1}^{1} x\,dx = 0 = w_1 x_1 + w_2 x_2$$

$$f(x) = x^2 \qquad \int_{-1}^{1} x^2 dx = 2/3 = w_1 x_1^2 + w_2 x_2^2$$

$$f(x) = x^3 \qquad \int_{-1}^{1} x^3 dx = 0 = w_1 x_1^3 + w_2 x_2^3$$

- This is a 4x4 nonlinear system

- A nonlinear system has to be quite special to be solvable.

- The above is!

$$w_1 = w_2 = 1$$

$$x_1 = -\frac{\sqrt{3}}{3} \qquad x_2 = \frac{\sqrt{3}}{3}$$

- easy to check the equations!
- $\int_{-1}^{1} f(x)\,dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$

is exact for polynomials of degree up to 4.

- Pretty Remarkable!

1777 – 1855

- Carl Friedrich Gauss managed to solve problems like that in great generality.
- How he did that is our next topic