Math 5610 Fall 2021

Notes of 10/28/21

- Monday: Discussion of hw 3
- Tuesday: Gaussian Quadrature, another brain storming session. Notes will appear after class.
- Video of Wednesday will appear today or this weekend.

Numerical Integration

- also called:

**Quadrature**

- We want to approximate

\[ I = \int_{a}^{b} f(x) \, dx. \]

- The basic idea underlying many techniques is to integrate the interpolating polynomial:

\[ \int_{a}^{b} f(x) \, dx \approx \int_{a}^{b} \sum_{i=0}^{n} f(x_i) L_i(x) \, dx = \sum_{i=0}^{n} w_i f(x_i) \]

- from Latin *quadratus*, square, squared
where the $L_i$ are the Lagrange basis functions and the weights or coefficients $w_i$ are given by

$$w_i = \int_a^b L_i(x) \, dx.$$

- If the $x_i$ are equally spaced throughout the interval of interest the resulting quadrature formulas are called **Newton-Cotes Formulas**. If the knots include the endpoints the formula is a closed Newton Cotes Formula, if they do not it’s an open Newton-Cotes Formula.

- For example, the **Trapezoidal Rule** is given by

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

- Doing the same for an interpolating quadratic gives **Simpson’s Rule**:

$$\int_a^{a+2h} f(x) \, dx \approx \frac{h}{3} (f(a) + 4f(a+h) + f(a+2h)).$$

- The Trapezoidal and Simpson’s Rules are the first two closed Newton-Cotes formulas.

- The first two open Newton-Cotes Formulas are the **midpoint rule**

$$\int_a^{a+2h} f(x) \, dx \approx 2hf(a + h)$$
and
\[ \int_{a}^{a+3h} f(x)\,dx \approx \frac{3h}{2} (f(a + h) + f(a + 2h)). \]
Method of Unknown Coefficients

• It’s a good exercise to derive Simpson’s Rule by actually integrating the Lagrange form of the interpolating quadratic.

• However, here is another idea for deriving quadrature rules and other formulas:

• Use knowledge of the properties of the formula to derive a set of simple equations that can be solved.

• For example, we know that Simpson’s Rule has the form

\[ \int_a^{a+2h} f(x) \, dx \approx h \left( Af(a) + Bf(a+h) + Cf(a+2h) \right) \]

• We also know that it gives the exact interval if \( f \) is a quadratic polynomial.

• So write down the formula for some special choices of \( a, h, \) and \( f \), and solve the resulting linear system.

• For example, for Simpson’s Rule the derivation becomes quite easy by choosing \( a = -1, \quad h = 1, \) and \( f = 1, x, x^2 \).

\[ \int_{-1}^{1} f(x) \, dx \approx \left( A f(-1) + B f(0) + C f(1) \right) \]
\[
\int_1^2 dx = 2 = A + B + C \implies B = \frac{4}{3}
\]
\[
\int x \, dx \geq 0 = -A + 0 + c \implies A = c
\]
\[
\int x^2 \, dx = \frac{2}{3} = A + 0 + C \implies A = c = \frac{1}{3}
\]
Error Analysis

- The basic idea is to expand the error

\[ E = \int_a^b f(x)dx - \sum_{i=1}^n w_i f(x_i) \]

into a Taylor series in \( h \).

- We’ll illustrate this for the Trapezoidal Rule:

\[
\begin{align*}
\int_a^{a+h} f(x)dx - \frac{h}{2} (f(a) + f(a+h)) &= \\
= F(a+h) - F - \frac{h}{2} (f + f(a+h)) &= \\
F + h F' + \frac{h^2}{2} F'' + \frac{h^3}{6} F''' + \cdots + \text{HOT} &= \\
- \frac{h}{2} \left( f + f + hf' + \frac{h^2}{2} f'' + \cdots \right) &= - \frac{h^3}{12} F' + \text{HOT}
\end{align*}
\]
and Simpson’s Rule

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

\[ = F + \frac{h}{2} F' + \frac{h^2}{6} F'' + \frac{h^3}{12} F''' + \frac{h^4}{24} F'''' + \frac{h^5}{120} F''''' + \frac{h^6}{720} F'''''' \]

\[ - \left( F - \frac{h}{2} F' + \frac{h^2}{6} F'' - \frac{h^3}{12} F''' + \frac{h^4}{24} F'''' + \frac{h^5}{120} F''''' - \frac{h^6}{720} F'''''' \right) \]

\[ - \frac{h}{3} \left( f - 6f' + 11f'' - 6f''' + f^{iv} \right) \]

\[ = h^5 \left( \frac{1}{120} - \frac{1}{720} \right) f^{iv} \]

\[ \frac{1}{60} - \frac{1}{36} = \frac{3 - 5}{180} = -\frac{1}{90} \]

\[ E = -\frac{1}{90} h^5 f^{iv} + \text{Hot} \]
We see that Simpson’s Method is **exact for cubics** even though it is obtained by interpolating a **quadratic** interpolant.

- How remarkable.

### Composite Newton-Cotes Formulas

- One could in principle integrate interpolating polynomials of high degree but as in the case of interpolation that’s not a good idea.

- It is better to apply low degree Newton-Cotes Formulas on subintervals.

- So let

\[ h = \frac{b - a}{N}, \quad x_n = a + nh, \quad n = 0, 1, \ldots, N \]

- Then the **composite Trapezoidal Rule** is given

\[
\int_a^b f(x) \, dx = \frac{h}{2} \left( f(a) + 2 \sum_{n=1}^{N-1} f(x_i) + f(b) \right) + E_T
\]

where

\[ E_T = -\frac{(b - a)h^2}{12} f''(\xi). \]

- The **composite Simpson’s Rule** (for even
\( N \) is given by
\[
\int_a^b f(x) \, dx = \frac{h}{3} \left( f(a) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \ldots + 4f(x_{N-1}) + f(b) \right) + E_S
\]

where
\[
E_S = -\frac{(b - a)h^4}{90} f^{iv}(\eta).
\]

Note that we loose one power of \( h \) as we go from the simple to the composite rule.

- Notice that we multiply the function values with positive coefficients.
- There is no cancellation of significant digits.
- However, as the polynomial degree goes up some of the coefficients become negative. For closed Newton-Cotes Formulas this first happens when \( n = 8 \).
- Formulas for closed Newton-Cotes Formula, for \( n = 1, 2, \ldots, 10 \), and open Newton-Cotes Formulas, for \( n = 1, 2, \ldots, 8 \) can be found on pages 886-887 of
- Note: Abramowitz/Stegun is still useful and widely used and quoted. However, there is a
successor which is organized quite differently:

- In all cases we obtain formulas of the form

\[ \int_a^b f(x)\,dx \approx \sum_{i=0}^{n} w_i f(x_i) \]

where the \( x_i \) are the knots, nodes, or abscissas and the \( w_i \) are the weights or coefficients.

- For Newton-Cotes Formulas the nodes are equally spaced and the coefficients are chosen so as to make the formula exact for polynomials of degree as high as possible.

- There is also a class of Chebyshev’s equal weight integration formulas where the weights are equal and the abscissas are chosen so as to make the formula exact for polynomials of degree \( n \). For \( n = 8 \) and \( n > 10 \) some of those abscissas are complex. For more information see Abramowitz/Stegun, p. 887.

- Equally spaced nodes make sense if we have data given in a Table.

- But if we can evaluate a function anywhere it makes more sense to pick the weights and the abscissas so as to get exactness for polynomials of degree as high as possible.
This gives rise to **Gaussian Quadrature** formulas.

Let’s illustrate the idea for \( n = 1 \) and \([a, b] = [-1, 1]\). We want to find a formula such that

\[
\int_{-1}^{1} f(x) dx \approx w_1 f(x_1) + w_2 f(x_2)
\]

which is exact if \( f \) is a polynomial of degree up to 3.

We get the **nonlinear** \( 4 \times 4 \) system:

\[
\begin{align*}
  f(x) &= 1 & \int_{-1}^{1} 1 dx &= 2 &= w_1 + w_2 \\
  f(x) &= x & \int_{-1}^{1} x dx &= 0 &= w_1 x_1 + w_2 x_2 \\
  f(x) &= x^2 & \int_{-1}^{1} x^2 dx &= 2/3 &= w_1 x_1^2 + w_2 x_2^2 \\
  f(x) &= x^3 & \int_{-1}^{1} x^3 dx &= 0 &= w_1 x_1^3 + w_2 x_2^3
\end{align*}
\]

In general, nonlinear systems can be very hard to solve.

However, it is easy to check that the system (1) has the solution

\[
\begin{align*}
  w_1 &= 1 \\
  w_2 &= 1 \\
  x_1 &= -\frac{\sqrt{3}}{3} \\
  x_2 &= \frac{\sqrt{3}}{3}
\end{align*}
\]
• This is pretty remarkable!

• Carl Friedrich Gauss (1777-1855) managed to solve problems like (1) in great generality.

• How he did this is our next topic.

• As for his analysis, we’ll try to develop his approach together, and I’ll put notes online only after class.