

Lecture 24

Simpson's Rule

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Today:

Objectives

- Review Trapezoid Rule
- Higher Order Interpolation Rules
Motivate Better Quadrature Rules
- Trapezoid Rule \rightarrow Simpson's Rule
- Composite Simpson's Rule
- General Newton-Cotes Rules

Material

- Section 11.2.2, 11.2.3

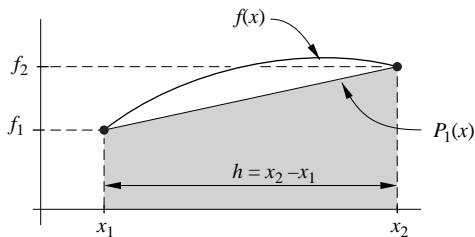
Basic Idea

- 1 Want to calculate the integral of some arbitrary function $f(x)$ over the interval $[x_1, x_2]$.
- 2 Approximate $f(x)$ with a Lagrange Polynomial, $P_n(x)$, of degree n .
- 3 Analytically integrate the interpolating polynomial to derive a quadrature rule.

Trapezoid Rule - Review

- Want to calculate the integral of $f(x)$ over the interval $[x_1, x_2]$.
- Draw a trapezoid defined by the two function points, (x_1, f_1) and (x_2, f_2) , and calculate the integral of the trapezoid.
- Trapezoid Rule:

$$\int_{x_1}^{x_2} f(x) dx \approx \int_{x_1}^{x_2} P_1(x) dx = \frac{1}{2}(f_1 + f_2)h$$



Trapezoid Derived

- Want to calculate the integral of $f(x)$ over the interval $[x_1, x_2]$.
- Approximate $f(x)$ with a linear Lagrange interpolating polynomial made from 2 points, (x_1, f_1) and (x_2, f_2) .
- Let

$$f(x) \approx P_1(x) = \frac{(x - x_2)}{(x_1 - x_2)}f_1 + \frac{(x - x_1)}{(x_2 - x_1)}f_2$$

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$$\int_{x_1}^{x_2} f(x) dx \approx \int_{x_1}^{x_2} P_1(x) dx = \frac{1}{2}(f_1 + f_2)h$$

Trapezoid Example

$$\int_{x_1}^{x_2} f(x) dx \approx \frac{1}{2}(f_1 + f_2)h, \text{ where } f(x) = 15x^2$$

Example

$$\begin{aligned}\int_1^2 15x^2 &\approx \frac{1}{2}(15 * 1^2 + 15 * 2^2) * 1 \\ &= \frac{1}{2}(15 + 60) = 37.5\end{aligned}$$

- Analytical answer is $\int_1^2 15x^2 = 5x^3 \Big|_1^2 = 40 - 5 = 35$.
- Truncation error for (the non-composite) Trapezoid Rule is in general of order $O(f''h^3)$, for step size, h . Note that the second derivative for $f(x)$ is not zero here, so we don't expect to have a zero error.

Simpson's Rule

Basic Idea

Problem: The approximation of the integral of some arbitrary function $f(x)$ over the interval $[x_1, x_3]$, where $x_3 = x_1 + 2h$, for step size h .

- Want a better integration rule than the Trapezoid Rule.
- Trapezoid Rule is based on linear interpolation of $f(x)$, so try higher order interpolation.

Solution: Simpson's Rule. Approximate $f(x)$ with a **Quadratic** interpolating Lagrange Polynomial, $P_2(x)$.

- Intuitively, quadratic interpolation should give us a better approximation to $f(x)$ and hence a better approximation to the integral of $f(x)$.

Simpson's Rule

Basic Idea Continued

- 1 Want to calculate the integral of some arbitrary function $f(x)$ over the interval $[x_1, x_3]$, where $x_3 = x_1 + 2h$, for step size h .
- 2 Approximate $f(x)$ with a **Quadratic** interpolating Lagrange Polynomial, $P_2(x)$.

$$f(x) \approx P_2(x)$$

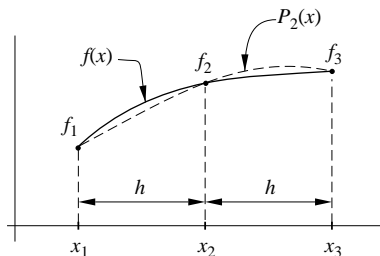
- ▶ Using quadratic interpolation implies that we will need three points over the interval of integration in order to uniquely define the quadratic interpolant.
 - ▶ Use the two endpoints, and the midpoint of the interval.
- 3 Analytically integrate the interpolating polynomial to derive a quadrature rule.

Simpson's Rule

Simpson's Rule for approximating the integral of a function, $f(x)$, over the interval $[x_1, x_3]$ is

$$\int_{x_1}^{x_3} f(x) dx \approx \int_{x_1}^{x_3} P_2(x) dx = h \left(\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3 \right)$$

- $x_3 = x_1 + 2h$ and $x_2 = x_1 + h$ for step size h .
- (x_1, f_1) and (x_3, f_3) are the end points of the interval.
- (x_2, f_2) is the midpoint of the interval.



Simpson's Rule

Example

$$\int_{x_1}^{x_3} f(x) dx \approx h \left(\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3 \right), \text{ where } f(x) = 15x^2$$

Example

$$\begin{aligned} \int_1^2 15x^2 &\approx 0.5 * \left(\frac{15 * 1^2}{3} + \frac{4 * 15 * 1.5^2}{3} + \frac{15 * 2^2}{3} \right) \\ &= 0.5 * (15/3 + 60 * 2.25/3 + 60/3) = 0.5 * (5 + 45 + 20) = 35 \end{aligned}$$

- Analytical answer is $\int_1^2 15 * x^2 = 5 * x^3 \Big|_1^2 = 40 - 5 = 35$.
- Compare with the answer from the Trapezoid Rule, which was 37.5.

Simpson's Rule

Derivation

- Approximate $f(x)$ with a quadratic Lagrange interpolating polynomial made from 3 points, (x_1, f_1) , (x_2, f_2) and (x_3, f_3) .
- Let

$$f(x) \approx P_2(x)$$
$$P_2(x) = \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)}f_1 + \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)}f_2 + \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)}f_3$$

- Multiply $P_2(x)$ out, let $x_2 = x_1 + h$, and $x_3 = x_1 + 2h$, simplify and then integrate analytically. The result is Simpson's Rule.

- $$\int_{x_1}^{x_2} f(x) dx \approx \int_{x_1}^{x_2} P_2(x) dx = h \left(\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3 \right)$$

Simpson's Rule

Truncation Error

Question: How many terms in the Taylor Series expansion of the integral match the Taylor Series expansion of Simpson's Rule exactly?

First, derive the Taylor Series expansion of the integral.

$$\int_{x_1}^{x_3} f(x) dx = \int_{x_1}^{x_1+2h} f(x) dx$$

Expand the $f(x)$ term under the integral sign around x_1 .

$$= \int_{x_1}^{x_1+2h} f_1 + (x - x_1)f_1' + \frac{(x - x_1)^2}{2!}f_1'' + \frac{(x - x_1)^3}{3!}f_1''' + \frac{(x - x_1)^4}{4!}f_1^{(4)} + \dots dx$$

Analytically integrate each individual term under the integral sign.

$$= 2hf_1 + 2h^2f_1' + \frac{4}{3}h^3f_1'' + \frac{2}{3}h^4f_1''' + \frac{2^5}{5 * 4!}h^5f_1^{(4)} + \dots$$

Simpson's Rule

Truncation Error Continued

Derive the Taylor Series expansion of Simpson's Rule, by expanding each point around x_1 .

① $f(x_1) = f_1$

② $f(x_2) = f(x_1 + h) = f_1 + hf_1' + \frac{h^2}{2!}f_1'' + \frac{h^3}{3!}f_1''' + \frac{h^4}{4!}f_1^{(4)} + \dots$

③ $f(x_3) = f(x_1 + 2h) = f_1 + 2hf_1' + \frac{(2h)^2}{2!}f_1'' + \frac{(2h)^3}{3!}f_1''' + \frac{(2h)^4}{4!}f_1^{(4)} + \dots$

Hence,

$$h \left(\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3 \right) =$$
$$2hf_1 + 2h^2f_1' + \frac{4}{3}h^3f_1'' + \frac{2}{3}h^4f_1''' + \frac{20}{3 * 4!}h^5f_1^{(4)} + \dots$$

Simpson's Rule

Truncation Error Concluded

Compare the Taylor Series Expansion for Simpson's Rule and the exact solution. The Truncation Error is the lowest order term which disagrees. Simpson's Rule gives us

$$h \left(\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3 \right) = \\ 2hf_1 + 2h^2f_1' + \frac{4}{3}h^3f_1'' + \frac{2}{3}h^4f_1''' + \frac{20}{3 * 4!}h^5f_1^{(4)} + \dots$$

The Exact Solution gives us

$$\int_{x_1}^{x_3} f(x) dx = \int_{x_1}^{x_1+2h} f(x) dx = \\ = 2hf_1 + 2h^2f_1' + \frac{4}{3}h^3f_1'' + \frac{2}{3}h^4f_1''' + \frac{2^5}{5 * 4!}h^5f_1^{(4)} + \dots$$

The Truncation Error is then,

$$O \left(\frac{h^5}{90} f_1^{(4)} \right)$$

Simpson's Rule

Example Revisited

$$\int_{x_1}^{x_3} f(x) dx \approx h \left(\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3 \right), \text{ where } f(x) = 15x^2$$

Example

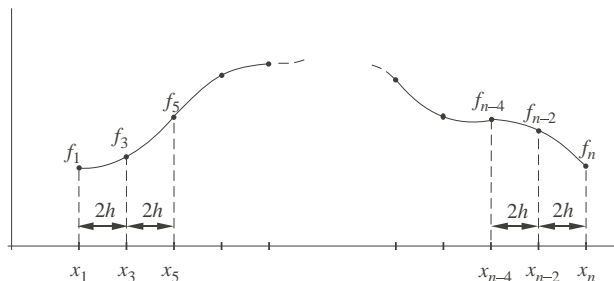
$$\begin{aligned} \int_1^2 15x^2 &\approx 0.5 * \left(\frac{15 * 1^2}{3} + \frac{4 * 15 * 1.5^2}{3} + \frac{15 * 2^2}{3} \right) \\ &= 0.5 * (15/3 + 60 * 2.25/3 + 60/3) = 0.5 * (5 + 45 + 20) = 35 \end{aligned}$$

- Analytical answer is $\int_1^2 15 * x^2 = 5 * x^3 \Big|_1^2 = 40 - 5 = 35$.
- Truncation Error for (the noncomposite) Simpson's Rule is in general of order $O(f^{(4)}h^5)$, for step size, h . The fourth derivative of $f(x) = 0$, so our error should be zero for this example.

Composite Simpson's Rule

General Idea

- Extend the idea of the Composite Trapezoid Rule.
- Take n equally spaced points inside of an arbitrary interval $[x_1, x_n]$.
- $(n - 1)$ must be even.
 - ▶ One application of Simpson's Rule requires 3 points, 2 applications requires 5 points, 3 applications require 7 points and so on.
- Step size is then $h = (x_n - x_1)/(n - 1)$.
- Composite rule is obtained by applying the basic Simpson's Rule on each subinterval, $[x_1, x_3]$, $[x_3, x_5]$, \dots , $[x_{n-2}, x_n]$.



Composite Simpson's Rule

Derivation

Apply Simpson's Rule multiple times

$$\begin{aligned}\int_{x_1}^{x_n} f(x) dx &\approx h \left(\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3 \right) + \\ &\quad h \left(\frac{1}{3}f_3 + \frac{4}{3}f_4 + \frac{1}{3}f_5 \right) + \\ &\quad \vdots \\ &\quad h \left(\frac{1}{3}f_{n-2} + \frac{4}{3}f_{n-1} + \frac{1}{3}f_n \right) \\ &= \frac{h}{3} [f_1 + 4f_2 + 2f_3 + 4f_4 + 2f_5 + \dots \\ &\quad + 2f_{n-4} + 4f_{n-3} + 2f_{n-2} + 4f_{n-1} + f_n]\end{aligned}$$

Composite Simpson's Rule

Derivation

Apply Simpson's Rule multiple times

$$\begin{aligned}\int_{x_1}^{x_n} f(x) dx &\approx \frac{h}{3} [f_1 + 4f_2 + 2f_3 + 4f_4 + 2f_5 + \dots \\ &\quad + 2f_{n-4} + 4f_{n-3} + 2f_{n-2} + 4f_{n-1} + f_n] \\ &= \frac{h}{3} \left[f_1 + \left(4 \sum_{i=2,4,\dots}^{n-1} f_i \right) + \left(2 \sum_{i=3,5,\dots}^{n-2} f_i \right) + f_n \right]\end{aligned}$$

Equivalent to the Matlab code:

```
Integral = f(1) + 4*sum(f(2:2:n-1)) + 2*sum(f(3:2:n-2)) + f(n);
```

Composite Simpson's Rule

Truncation Error

Add in Truncation Error terms to above derivation

$$\begin{aligned}\int_{x_1}^{x_n} f(x) dx &= h \left(\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3 \right) + O\left(\frac{h^5}{90}f_1^{(4)}\right) \\ &\quad h \left(\frac{1}{3}f_3 + \frac{4}{3}f_4 + \frac{1}{3}f_5 \right) + O\left(\frac{h^5}{90}f_3^{(4)}\right) \\ &\quad \vdots \\ &\quad h \left(\frac{1}{3}f_{n-2} + \frac{4}{3}f_{n-1} + \frac{1}{3}f_n + O\left(\frac{h^5}{90}f_{n-2}^{(4)}\right) \right)\end{aligned}$$

- 1 Let $K = \max\left(\frac{1}{90}f^{(4)}\right)$ and $K' = K * (x_n - x_1)$.
- 2 Sum the error terms to find the Truncation Error of Composite Rule,

$$\begin{aligned}O((n-1) * K * h^5) &\rightarrow O\left((n-1) * K * \left(\frac{x_n - x_1}{n-1}\right)^5\right) \rightarrow \\ O\left(K * \frac{(x_n - x_1)^5}{(n-1)^4}\right) &\rightarrow \mathbf{O(K'h^4)}\end{aligned}$$

Composite Simpson's Rule

Example

Example

$$\begin{aligned} I &= \frac{2}{\sqrt{\pi}} \int_0^1 e^{-x^2} dx \\ &= \frac{2}{\sqrt{\pi}} \frac{0.25}{3} [1.0 + 4(0.9394) + 2(0.778) + 4(0.5698) + 0.3679] \\ &= 0.8427 \end{aligned}$$

- The error, with $n = 5$, is 0.0001.
 - ▶ $n = 5$ yields 2 applications of Simpson's Rule
- For the same number of evaluations of $f(x)$, the Trapezoid Rule results in an error of -0.0043.
 - ▶ See page 606 for the application of the Trapezoid Rule to this function.

Simpson's Rule

Matlab Examples

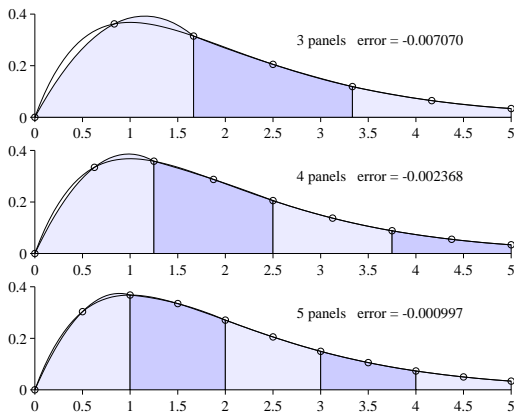
- Code: *simpson.m* and *xemx.m*
- *xemx.m* is just a function, $f(x) = x e^{-x}$.
- *simpson.m* implements the Composite Simpson's Rule
 - ▶ Call with *simpson(fun, a, b, nPanels)*
 - ▶ *fun* is an inline function or a string that is the name of an m-file. For the m-file, *class257.m*, *fun = 'class257'*; drop the *.m*.
 - ▶ *a* and *b* are the endpoints of the interval of integration.
 - ▶ *nPanels* is the number of panels to use in the integration.
Total number of nodes = $2 * nPanels + 1$.

Code is courtesy of NMM's website.

Simpson's Rule

Matlab Examples Continued

- Problem: $\int_0^5 x e^{-x} dx$
- Code: `demoSimp.m`, which uses `xemx.m` and `simpson.m`
- Note how the quadratic interpolant handles the hump on the left well. How well would a linear interpolant work?



Recap

- 1 We started with the Trapezoid Rule, which numerically integrates a function by integrating a linear interpolant of the function.
- 2 Using knowledge from the interpolation chapter that better interpolants than linears exist, we numerically integrate the function by integrating a quadratic interpolant of the function. This gives us Simpson's Rule.
 - ▶ Simpson's Rule has 2 more orders of accuracy than the Trapezoid Rule.
 - ▶ Note that Simpson's Rule uses a quadratic interpolant, but integrates cubics exactly. This seemingly counterintuitive result is from fortuitous cancellation of Taylor Series terms. Remember that the error is of order $O\left(\frac{h^5}{90}f_1^{(4)}\right)$, so any function whose fourth and higher derivatives are 0, is integrated exactly.
- 3 Why not use even higher order interpolants to get even more accurate quadrature rules?

Newton-Cotes Quadrature

General Idea

Build on the idea of using higher order polynomial interpolants of functions to numerically integrate functions.

Integrating an n -degree interpolant, which has $(n + 1)$ evenly spaced points as its knots, yields an $(n + 1)$ point Newton-Cotes Integration Rule. We've already seen two such rules with the Trapezoid Rule and Simpson's Rule.

- 1 Trapezoid Rule is

$$\int_{x_1}^{x_2} f(x) dx \approx \int_{x_1}^{x_2} P_1(x) dx = \frac{1}{2}(f_1 + f_2)h$$

- 2 Simpson's Rule is

$$\int_{x_1}^{x_3} f(x) dx \approx \int_{x_1}^{x_3} P_2(x) dx = h \left(\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3 \right)$$

Newton-Cotes Quadrature

Examples

Two more Newton-Cotes Rules are

- 1 Simpson's 3/8 rule

$$\int_{x_1}^{x_4} f(x) dx \approx \int_{x_1}^{x_4} P_3(x) dx = \frac{3}{8}h(f_1 + 3f_2 + 3f_3 + f_4)$$

- 2 6 Point rule

$$\int_{x_1}^{x_6} f(x) dx \approx \int_{x_1}^{x_6} P_5(x) dx = \frac{5}{288}h(19f_1 + 75f_2 + 50f_3 + 50f_4 + 75f_5 + 19f_6)$$

Many more Newton-Cotes rules exist, but for stability reasons, rules of order greater than 11 aren't normally used.