

Lecture 11 - B

§5.1, 5.3 Newton-Cotes

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Goals

We will answer these questions:

- How accurate is Trapezoid method?
- What is Simpson's rule and how accurate is it?
- What are Newton-Cotes rules and how are they related to splines?



Interpolation Review

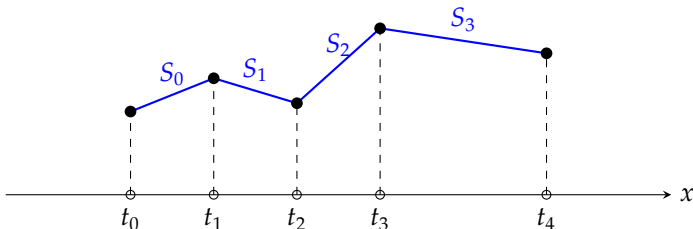


First-Degree Spline

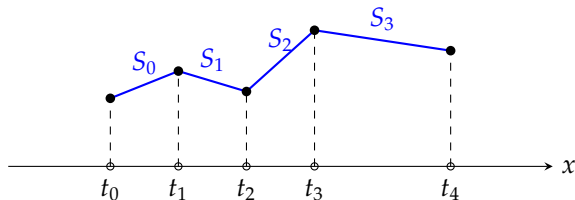
Definition: First-Degree Spline

A function $S(x)$ is a **spline of degree 1** if it satisfies all of the following:

- 1 The domain of $S(x)$ is an interval $[a, b]$
- 2 $S(x)$ is continuous on $[a, b]$
- 3 There is a partition $a = t_0 < t_1 < \cdots < t_n = b$ such that $S(x)$ is linear on each subinterval $[t_i, t_{i+1}]$.



Linear Approximation

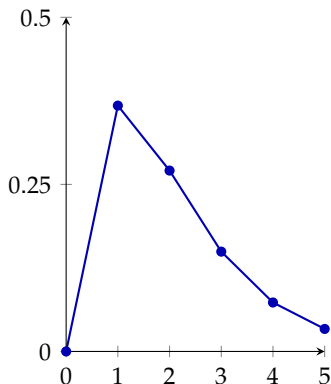
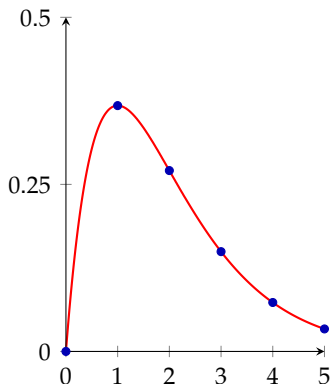


- Each piece of the spline is a linear function

$$S_i(x) = a_i x + b_i$$



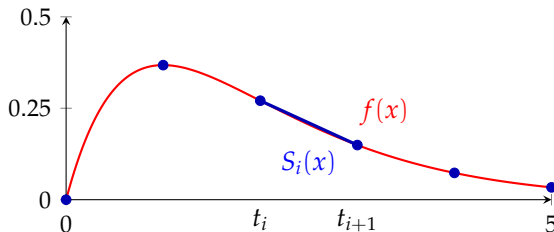
Approximating Functions



- A function can be sampled and approximated with a degree one spline



Interpolation Error



Degree One Spline Error

We know the error on each spline piece

$$e_i(x) = f(x) - S_i(x) = \frac{(x - t_i)(x - t_{i+1})}{2} f''(c)$$



Trapezoid Error Analysis



Truth about Trapezoid Method

Here's the truth about trapezoid method

Trapezoid method is actually just:

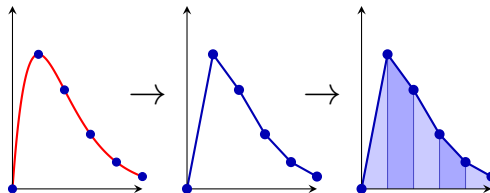


Truth about Trapezoid Method

Here's the truth about trapezoid method

Trapezoid method is actually just:

- 1 Approximating $f(x)$ with a degree 1 spline $S(x)$,
- 2 Then integrating the spline $\int S(x) dx$



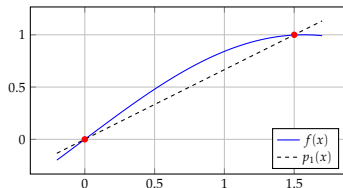
Why does that matter?

Question

Why is it useful to think of it as the integral of a degree 1 spline?

- We know the interpolation error

$$e_1(x) = f(x) - p_1(x) = \frac{(x - x_0)(x - x_1)}{2} f''(c)$$

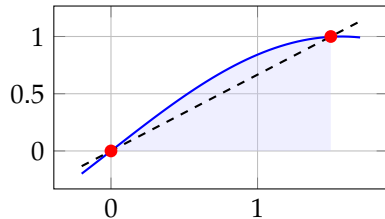


Key Idea

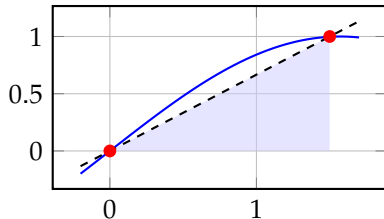
We may use the interpolation error formula.

Trapezoid Error

Illustration



$$I = \int_a^b f(x) dx$$



$$T = \int_a^b p_1(x) dx$$

Trapezoid Error

$$E = I - T = \int_a^b f(x) dx - \int_a^b p_1(x) dx$$



Accuracy for Basic Trapezoid

Part 1

- Substitute the interpolation error

$$f(x) - p_1(x) = \frac{(x - x_0)(x - x_1)}{2} f''(c)$$

- into the integration error equation

$$\begin{aligned} E &= \int_a^b f(x) dx - \int_a^b p_1(x) dx = \int_a^b (f(x) - p_1(x)) dx \\ &= \frac{1}{2} \int_a^b f''(c)(x - a)(x - b) dx \quad (\text{note } (x - a)(x - b) \geq 0 \text{ in } [a, b]) \\ &= \frac{f''(c)}{2} \int_a^b (x - a)(x - b) dx \end{aligned}$$



Accuracy for Basic Trapezoid

Part 2

- Integration by parts, $u = (x - b)$ and $dv = (x - a) dx$

$$\begin{aligned} E &= \frac{f''(c)}{2} \int_a^b (x - a)(x - b) dx \\ &= \frac{f''(c)}{2} \left(\frac{1}{2}(x - a)(x - b) \Big|_a^b - \frac{1}{2} \int_a^b (x - a)^2 dx \right) \\ &= \frac{f''(c)}{2} \left(-\frac{1}{6}(b - a)^3 \right) \\ &= -\frac{(b - a)^3 f''(c)}{12} \end{aligned}$$

Question

This is the error for basic trapezoid. What about the composite trapezoid?

Accuracy for Composite Trapezoid

Part 1

- Composite Trapezoid is just basic trapezoid n times

$$T_{\text{comp}} = \int_a^b f(x) dx \approx \sum_{i=0}^{n-1} T_i$$

- The error in each interval $[x_i, x_{i+1}]$ is

$$E_i = \int_{t_i}^{t_{i+1}} f(x) dx - T_i = -\frac{(x_{i+1} - x_i)^3 f''(c)}{12} = -\frac{h^3 f''(c_i)}{12}$$

- The **total error** can be derived by adding up each error

$$E_{\text{comp}} = \sum_{i=0}^{n-1} E_i = \sum_{i=0}^{n-1} -\frac{h^3 f''(c_i)}{12}$$



Accuracy for Composite Trapezoid

Part 2

- Let's define the average value of $f(c_i)$

$$f''(c) = \sum_{i=0}^{n-1} \frac{f''(c_i)}{n}$$

- Now we can manipulate the total error by multiplying by $\frac{n}{n}$

$$\begin{aligned} E_{\text{comp}} &= \sum_{i=0}^{n-1} -\frac{h^3 f''(c_i)}{12} \frac{n}{n} \\ &= -n \frac{h^3}{12} \sum_{i=0}^{n-1} \frac{f''(c_i)}{n} \\ &= \frac{-nh^3}{12} f''(c) \end{aligned}$$

- Finally, use the fact that $n = \frac{b-a}{h}$

$$E_{\text{comp}} = \frac{-nh^3}{12} f''(c) = -\frac{(b-a)h^2 f''(c)}{12}$$



Trapezoid Error

Basic Trapezoidal Rule Error

$$E = -\frac{(b-a)^3 f''(c)}{12}$$

Composite Trapezoidal Rule Error

$$E_{\text{comp}} = -\frac{(b-a)h^2 f''(c)}{12} = \mathcal{O}(h^2)$$

- n = number of subintervals, h = width of trapezoids
- As $n \rightarrow \infty$, the error goes to zero quadratically
- We can use the error theorem to find appropriate n



Using the Error Theorem

Example

What value of n will ensure the composite Trapezoid rule is accurate to $\epsilon = 10^{-6}$ for $\int_0^1 e^{-x^2} dx$?

- Set up the inequality $E < \epsilon$

$$\frac{(b-a)h^2 f''(c)}{12} \leq 10^{-6}$$

- Find worst case scenario for $f''(c)$

$$f(x) = e^{-x^2}$$

$$f'(x) = -2xe^{-x^2}$$

$$f''(x) = -2e^{-x^2} + 4x^2 e^{-x^2} = 2e^{-x^2}(2x^2 - 1)$$

$$f'''(x) = 12xe^{-x^2} - 8x^3 e^{-x^2} = xe^{-x^2}(12 - 8x^2)$$

f''' is always positive so f'' is monotone increasing and thus f'' takes on a maximum at 0: $f''(0) = -2 \Rightarrow |f''(c)| \leq 2$.

- Finally we solve for n

$$E = \frac{(b-a)2h^2}{12} = \frac{(b-a)^3}{6n^2} = \frac{1}{6n^2} \leq 10^{-6}$$

$$n^2 \geq 10^6/6 \Rightarrow n \geq 10^3/\sqrt{6} \approx 408.2$$



How do we improve Trapezoid?

- Riemann Sum = integrate degree ZERO spline
- Composite Trapezoid = integrate degree ONE spline

How do you improve?



How do we improve Trapezoid?

- Riemann Sum = integrate degree ZERO spline
- Composite Trapezoid = integrate degree ONE spline

How do you improve?

- Integrate a degree TWO spline

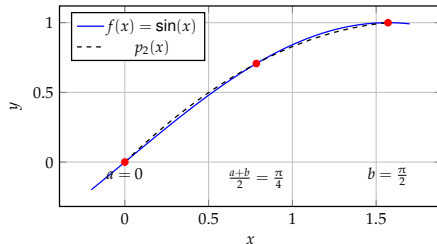


Simpson's Rule



Basic Simpson

The Idea



Steps:

- 1 Approximate $f(x)$ with a quadratic $p_2(x)$
- 2 Approximate $\int f(x) dx \approx \int p_2(x) dx$

Key Idea

Simpson's rule says integrate the quadratic interpolation $p_2(x)$ rather than the actual function.

Basic Simpson Derivation

Part 1

The goal is to approximate Consider $\int_a^b f(x) dx$

- Let $h = \frac{b-a}{2}$. Then partition $P = \{a, a+h, b = a+2h\}$
- To simplify things, consider $\int_0^{2h} f(x) dx$ so partition $P = \{0, h, 2h\}$
- Use Newton Divided difference to find $p_2(x)$:

$$\begin{aligned} f(x) &\approx p_2(x) \\ &= a_0 + a_1x + a_2x(x-h) \end{aligned}$$

- The coefficients are

$$a_0 = f[0] = f(0)$$

$$a_1 = f[0, h] = \frac{f(h) - f(0)}{h}$$

$$a_2 = f[0, h, 2h] = \frac{\frac{f(2h) - f(h)}{h} - \frac{f(h) - f(0)}{h}}{2h} = \frac{f(2h) - 2f(h) + f(0)}{2h^2}$$



Basic Simpson Derivation

Part 2

- The Newton interpolation is

$$f(x) \approx p_2(x) = f(0) + \frac{f(h) - f(0)}{h}x + \frac{f(2h) - 2f(h) + f(0)}{2h^2}x(x-h)$$

- Now integrate $\int_0^{2h} p_2(x) dx$ to get the basic Simpson's formula

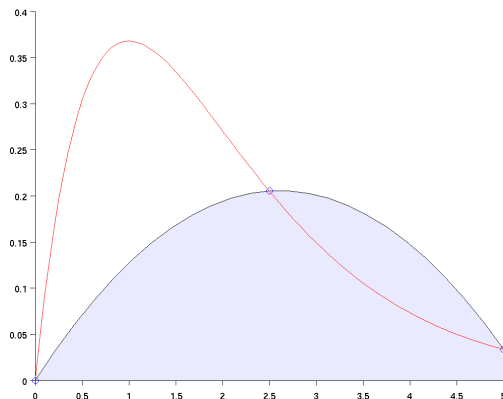
$$\begin{aligned}\int_0^{2h} p_2(x) dx &= \int_0^{2h} f(0) + \frac{f(h) - f(0)}{h}x + \frac{f(2h) - 2f(h) + f(0)}{2h^2}x(x-h) dx \\&= 2hf(0) + \frac{f(h) - f(0)}{h}(2h^2) + \frac{f(2h) - 2f(h) + f(0)}{2h^2} \frac{2h^3}{3} \\&= f(0) \left[2h - 2h + \frac{h}{3} \right] + f(h) \left[2h - \frac{2h}{3} \right] + f(2h) \left[\frac{h}{3} \right] \\&= \frac{h}{3} [f(0) + 4f(h) + f(2h)] \\&= \frac{2h}{6} [f(0) + 4f(h) + f(2h)]\end{aligned}$$



Basic Simpson

Basic Simpson's Rule

$$\int_a^b f(x) dx \approx \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$



Using Simpson's Rule Twice for one Interval

Question

How would you use the basic Simpson's rule twice under one interval $[a, b]$?

- You would have to divide $[a, b]$ into 4 even subintervals with nodes

$$\{x_0 = a, x_1, x_2, x_3, x_4 = b\}$$

- The first Simpson's rule approximates integral over $\{x_0, x_1, x_2\}$

$$I_0 = \int_{x_0}^{x_2} S_0(x) dx = \frac{x_2 - x_0}{6} [f(x_0) + 4f(x_1) + f(x_2)]$$

- The second Simpson's rule approximates integral over $\{x_2, x_3, x_4\}$

$$I_1 = \int_{x_2}^{x_4} S_0(x) dx = \frac{x_4 - x_2}{6} [f(x_2) + 4f(x_3) + f(x_4)]$$

- When we combine the two..

$$\begin{aligned} I_0 + I_1 &= \frac{x_2 - x_0}{6} [f(x_0) + 4f(x_1) + f(x_2)] + \frac{x_4 - x_2}{6} [f(x_2) + 4f(x_3) + f(x_4)] \\ &= \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] + \frac{h}{3} [f(x_2) + 4f(x_3) + f(x_4)] \\ &= \frac{h}{3} [f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(x_4)] \end{aligned}$$



Composite Simpson

- Divide $[a, b]$ into n subintervals, n must be an even number
- Apply basic Simpson's Rule over groups of 2 subintervals $[x_{2i}, x_{2i+2}]$

$$\begin{aligned}\int_a^b f(x) dx &= \sum_{i=0}^{n/2-1} \int_{x_{2i}}^{x_{2i+2}} f(x) dx \\&= \sum_{i=0}^{n/2-1} \frac{2h}{6} [f(x_{2i}) + 4f(x_{2i+1}) + f(x_{2i+2})] \\&= \frac{h}{3} [f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots \\&\quad 4f(x_{n-1}) + f(x_n)]\end{aligned}$$

- Inner coefficients alternate between 4 and 2.



Composite Simpson

Formula

Composite Simpson's Rule

$$\int_a^b f(x) dx \approx \frac{h}{3} \left[f(a) + 4 \sum_{i=1}^{n/2} f(a + (2i-1)h) + 2 \sum_{i=1}^{n/2-1} f(a + 2ih) + f(b) \right]$$

Alternate Formula

$$\int_a^b f(x) dx \approx \frac{h}{3} \left[f(x_0) + 4 \left(\sum_{i \in [1, n-1]}^{i \text{ is odd}} f(x_i) \right) + 2 \left(\sum_{i \in [2, n-1]}^{i \text{ is even}} f(x_i) \right) + f(x_n) \right]$$

- The odd nodes $2i - 1$ have weight 4
- The even nodes $2i$ have weight 2
- The endpoints have weight 1

Composite Simpson

The method

Method: Uniform Composite Simpson's Method

- **Given:** Continuous function $f(x)$, interval $[a, b]$, an even number of subintervals n
- **Output:** Approximation to $\int_a^b f(x) dx$
- **Idea:** T

The integration of a degree 2 spline is more accurate than the Trapezoid Method, and it has a compact formula.

$$\int_a^b f(x) dx \approx \frac{h}{3} \left[f(x_0) + 4 \left(\sum_{i \in [1, n-1]}^{i \text{ is odd}} f(x_i) \right) + 2 \left(\sum_{i \in [2, n-1]}^{i \text{ is even}} f(x_i) \right) + f(x_n) \right]$$

$$n \text{ is even, } h = \frac{b-a}{n}$$



Simpson Error Analysis



Composite Simpson

Numerical Test

Question

How does Composite Simpson performs in terms of h ?

- Composite Trapezoid has order 2 convergence:

$$E_{\text{trap}} = \mathcal{O}(h^2)$$

- We can guess that

$$E_{\text{simp}} = \mathcal{O}(h^p)$$

- Run the experiment `simpson_int_test.m`



Composite Simpson

Numerical Test

Question

How does Composite Simpson performs in terms of h ?

- Composite Trapezoid has order 2 convergence:

$$E_{\text{trap}} = \mathcal{O}(h^2)$$

- We can guess that

$$E_{\text{simp}} = \mathcal{O}(h^p)$$

- Run the experiment `simpson_int_test.m`
- We get $p = 4$?



Analysis is Needed

- Consider the integral

$$\int_a^b f(x) dx$$

- Let $h = (b - a)/2$ so that

$$a = a, \quad \frac{a+b}{2} = a + h, \quad b = a + 2h$$

- Then the Simpson approximation is

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

Goal

We will study the error for Simpson's by Taylor expanding $f(x)$ around $x = a$.



Basic Simpson Error

Part 1

- First, Taylor expand around a

$$f(a) = f$$

$$f(a+h) = f + hf' + \frac{1}{2!}h^2f'' + \frac{1}{3!}h^3f''' + \frac{1}{4!}h^4f^{(4)} + \frac{1}{5!}h^5f^{(5)} + \dots$$

$$f(a+2h) = f + 2hf' + 2h^2f'' + \frac{4}{3}h^3f''' + \frac{2}{3}h^4f^{(4)} + \frac{4}{15}h^5f^{(5)} + \dots$$

- This gives

$$\frac{h}{3} [f(a) + 4f(a+h) + f(a+2h)] = 2hf + 2h^2f' + \frac{4}{3}h^3f'' + \frac{2}{3}h^4f''' + \frac{5}{18}h^5f^{(4)}$$



Basic Simpson Error

Part 2

- Consider the antiderivative of $f(x)$:

$$F(x) = \int_a^x f(t) dt$$

- Taylor series of F :

$$F(a+2h) = F(a) + 2hF'(a) + 2h^2F''(a) + \frac{4}{3}h^3F'''(a) + \frac{2}{3}h^4F^{(4)}(a) + \frac{4}{15}h^5F^{(5)}(a) + \dots$$

- Noting that $F(a+2h) = \int_a^{b=a+2h} f(x) dx$, $F(a) = 0$, $F' = f$, $F'' = f'$ and so on,

$$\int_a^{b=a+2h} f(x) dx = 2hf + 2h^2f' + \frac{4}{3}h^3f'' + \frac{2}{3}h^4f''' + \frac{4}{15}h^5f^{(4)} + \dots$$



Basic Simpson Error

Part 3

- The true value is

$$\int_a^{b=a+2h} f(x) dx = 2hf + 2h^2f' + \frac{4}{3}h^3f'' + \frac{2}{3}h^4f''' + \frac{4}{15}h^5f^{(4)} + \dots$$

- The approximation is

$$\frac{h}{3} [f(a) + 4f(a+h) + f(a+2h)] = 2hf + 2h^2f' + \frac{4}{3}h^3f'' + \frac{2}{3}h^4f''' + \frac{5}{18}h^5f^{(4)}$$

- Thus, the error (their difference) is

Basic Simpson's Error

$$-\frac{1}{90} \left(\frac{b-a}{2} \right)^5 f^{(4)}(\xi)$$



Why is composite Simpson $\mathcal{O}(h^4)$?

- Error for one interval using basic Simpson's Rule:

$$-\frac{1}{90} \left(\frac{b-a}{2} \right)^5 f^{(4)}(\xi)$$

- Over $n/2$ subintervals $[x_{2i}, x_{2i+2}]$, the error adds up to

$$\begin{aligned} \text{err} &= \sum_{i=1}^{n/2} -\frac{1}{90} \left(\frac{x_{2i+2} - x_{2i}}{2} \right)^5 f^{(4)}(\xi_i) = -\frac{1}{90} \sum_{i=1}^{n/2} \left(\frac{2h}{2} \right)^5 f^{(4)}(\xi_i) \\ &= -\frac{1}{90} \frac{n}{2} h^5 f^{(4)}(\xi) = -\frac{1}{180} \frac{(b-a)}{h} h^5 f^{(4)}(\xi) \\ &= -\frac{b-a}{180} h^4 f^{(4)}(\xi) \end{aligned}$$

Composite Simpson's Rule Error

$$-\frac{b-a}{180} h^4 f^{(4)}(\xi)$$

We “gain” two orders over Trapezoid – got lucky!

Summary

Notice the pattern in our integration methods:

Method	Description	Accuracy
Left/Right Riemann	Approximate $f(x) \approx p_0(x)$ and integrate	$\mathcal{O}(h)$
Trapezoid	Approximate $f(x) \approx p_1(x)$ and integrate	$\mathcal{O}(h^2)$
Simpson	Approximate $f(x) \approx p_2(x)$ and integrate	$\mathcal{O}(h^4)$

Trapezoid and Simpson's both belong to a more general class of algorithms.



Newton-Cotes Formulas



Going Further

Method	Description	Accuracy
Left/Right Riemann	$\int f(x) \approx \int p_0(x)$	$\mathcal{O}(h)$
Trapezoid	$\int f(x) \approx \int p_1(x)$	$\mathcal{O}(h^2)$
Simpson	$\int f(x) \approx \int p_2(x)$	$\mathcal{O}(h^4)$

Question

What's stopping us from going further: $\int p_3(x)$, $\int p_4(x)$, ...?



Method: Newton-Cotes

- **Given:** $f(x)$, interval $[a, b]$
- **Output:** Approximation to $\int_a^b f(x) dx$
- **Idea:** Integrate the n^{th} degree interpolation $\int_a^b f(x) dx \approx \int_a^b p_n(x) dx$

Properties:

- The nodes x_i are equally spaced out
- Have the form $\int_a^b f(x) dx \approx \sum_{i=1}^n w_i f(x_i)$
- If $f(x)$ is an n^{th} degree polynomial, then error is **zero**



First Four Newton-Cotes Formulas

Basic Newton-Cotes rules:

name	n	formula
Trapezoid	1	$\frac{(b-a)}{2} [f(a) + f(b)]$
Simpson's 1/3	2	$\frac{(b-a)}{6} [f(a) + 4f(\frac{a+b}{2}) + f(b)]$
Simpson's 3/8	3	$\frac{(b-a)}{8} [f(a) + 3f(a+h) + 3f(b-h) + f(b)]$
Boole's	4	$\frac{(b-a)}{90} [7f(a) + 32f(a+h) + 12f(\frac{a+b}{2}) + 32f(b-h) + 7f(b)]$

Error bounds for composite Newton-Cotes:

name	n	error	h
Trapezoid	1	$-\frac{(b-a)h^2}{12} f''(\xi)$	$h = b - a$
Simpson's 1/3	2	$-\frac{(b-a)h^4}{90} f^{(4)}(\xi)$	$h = (b - a)/2$
Simpson's 3/8	3	$-\frac{(b-a)h^4}{80} f^{(4)}(\xi)$	$h = (b - a)/3$
Boole's	4	$-\frac{2(b-a)h^6}{945} f^{(6)}(\xi)$	$h = (b - a)/4$



Error bounds for composite Newton-Cotes:

name	n	error	h
Trapezoid	1	$-\frac{(b-a)h^2}{12}f''(\xi)$	$h = b - a$
Simpson's 1/3	2	$-\frac{(b-a)h^4}{90}f^{(4)}(\xi)$	$h = (b - a)/2$
Simpson's 3/8	3	$-\frac{(b-a)h^4}{80}f^{(4)}(\xi)$	$h = (b - a)/3$
Boole's	4	$-\frac{2(b-a)h^6}{945}f^{(6)}(\xi)$	$h = (b - a)/4$

- Notice that Simpson's 1/3 and Simpson's 3/8 are both $\mathcal{O}(h^4)$
- There is no advantage going from degree 2 spline to degree 3 spline



Pattern to the Formulas

Basic Newton-Cotes rules:

name	n	formula
Trapezoid	1	$\frac{(b-a)}{2} [f(a) + f(b)]$
Simpson's 1/3	2	$\frac{(b-a)}{6} [f(a) + 4f(\frac{a+b}{2}) + f(b)]$
Simpson's 3/8	3	$\frac{(b-a)}{8} [f(a) + 3f(a+h) + 3f(b-h) + f(b)]$
Boole's	4	$\frac{(b-a)}{90} [7f(a) + 32f(a+h) + 12f(\frac{a+b}{2}) + 32f(b-h) + 7f(b)]$

- There is a pattern to all of the formulas
- Let $a = x_0$, $b = x_n$, $h = \frac{b-a}{n}$, and $x_i = x_0 + ih$
- All of the formulas have the form

$$\sum_{i=0}^n w_i f(x_i)$$



- There is a reference book for many Newton-Cotes formulas
- There are also “Open” Newton-Cotes rules that do not use nodes at endpoints
 - Midpoint rule is an example, composite midpoint is $\mathcal{O}(h^2)$
- All formulas have a simple form making them easy to implement

$$\sum_{i=0}^n w_i f(x_i)$$

- More preferable to do a composite Newton-Cotes with smaller n
 - Two Composite Simpson’s rule $>$ One Basic Boole’s rule
- Used to be the most commonly used type of numerical integration
 - We will learn Gaussian quadratures next

