Lecture 16

Integration: Newton Cotes

David Semeraro

University of Illinois at Urbana-Champaign

October 22, 2013

Next...

- We can interpolate $f(x)$
- Can we integrate $f(x)$?

Why?

- Often $f(x)$ is only known implicitly (known at a certain number of points)
- Often the anti-derivative of $f(x)$ is not known.

Integrals

We seek a solution to the following quantity

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

The Fundamental Theorem of Calculus states that

$$\int_a^b f(x)\,dx = F(b) - F(a)$$

where F is the antiderivative of f. We don't know F, so we approximate the integral operation.

Integration

What is the integral $\int_a^b$?

- Let P be a partition of $[a, b]$ of $n + 1$ distinct and ordered points with $x_0 = a$ and $x_n = b$.
- For interval $[x_i, x_{i+1}]$ let m_i be a lower bound on $f(x)$
- For interval $[x_i, x_{i+1}]$ let M_i be an upper bound on $f(x)$
- Lower Sum:

$$L(f; P) = \sum_{i=0}^{n-1} m_i(x_{i+1} - x_i)$$

- Upper Sum:

$$U(f; P) = \sum_{i=0}^{n-1} M_i(x_{i+1} - x_i)$$

Integration

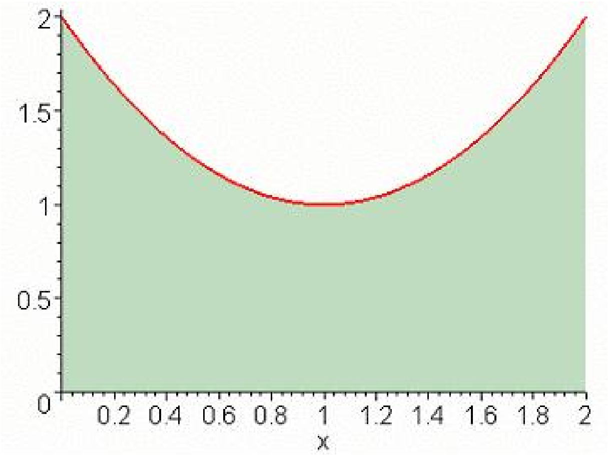
- The lower sum always under-approximates the integral
- The upper sum always over-approximates the integral

$$L(f;P) \leqslant \int_a^b f(x)\,dx \leqslant U(f;P)$$

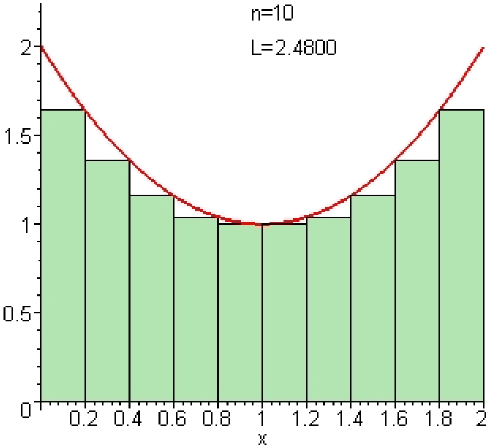
- In the limit, they are equal

$$\lim_{n\to\infty} L(f;P) = \int_a^b f(x)\,dx = \lim_{n\to\infty} U(f;P)$$

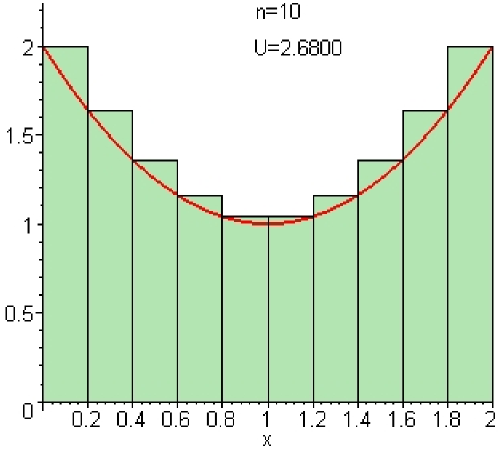
Graphically: Integral



Graphically: Lower sum



Graphically: Upper sum



Left-Riemann, Right-Riemann, Mid-Point

- The upper and lower bounds are often difficult to identify
- Use Left-Riemann, Right-Riemann, and Middle Riemann Sums
- Generally the Riemann sum is

$$S = \sum_{i=0}^{n-1} f(z_i)(x_{i+1} - x_i)$$

  for $x_i \leqslant z_i \leqslant x_{i+1}$
- $z_i = x_i$ is a Left Riemann Sum
- $z_i = x_{i+1}$ is a Right Riemann Sum
- $z_i = \frac{x_{i+1} + x_i}{2}$ is a Middle Riemann Sum

Goals

We have a way to compute integrals. Why aren't we done?
We may need to compute zillions of integrals or we may need to accurately compute integrals in very short times to meet a real-time requirement.

- Trapezoid Rule
- Composite Trapezoid Rule
- Simpson Rule
- Composite Simpson Rule
- Newton-Cotes in general
- Section 5.2 in NMC

Trapezoid

Goal: Approximate

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

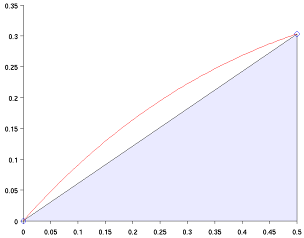
Goal: Approximate area under $f(x)$.

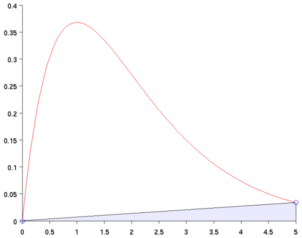
- Old Idea: Left,Right,Midpoint Riemann integration approximate $f(x)$ by a constant function and obtain the area under the constant function.
- New Idea: Trapezoid approximates $f(x)$ by a linear function (degree one polynomial) and obtains the area under the linear function.

Basic Trapezoid

Use endpoints $[a, b]$ to obtain a linear approximation to $f(x)$. The area under this function is the area of a trapezoid:

$$\int_a^b f(x)\,dx \approx \frac{1}{2}(b-a)(f(a)+f(b))$$





Basic Trapezoid

- Trapezoid Rule:

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

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

Example

$$\int_1^2 15\,x^2 \approx \frac{1}{2}(15 * 1^2 + 15 * 2^2) * 1$$

$$= \frac{1}{2}(15 + 60) = 37.5$$

- Analytical answer is $\int_1^2 15\,x^2 = 5\,x^3\big|_1^2 = 40 - 5 = 35.$

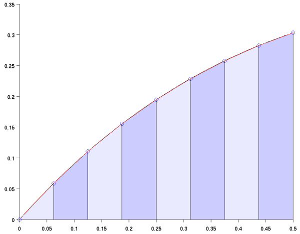
Composite Trapezoid

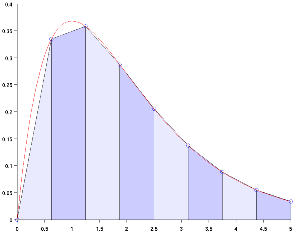
Obviously a naive linear approximation won't cut it.

Consider a partition $P = \{x_0 = a < \ldots x_n = b\}$ of $[a, b]$.

In each interval $[x_i, x_{i+1}]$ use the basic Trapezoid:

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n-1} \frac{1}{2}(x_{i+1} - x_i)(f(x_i) + f(x_{i+1}))$$





Composite Trapezoid

- With uniform spacing of P, $h_i = x_{i+1} - x_i = h$ is constant

$$T(f;P) = \int_a^b f(x)\,dx \approx \frac{h}{2}\sum_{i=0}^{n-1} f(x_i) + f(x_{i+1})$$

- This becomes

$$T(f;P) = \int_a^b f(x)\,dx \approx \frac{h}{2}\left(f(x_0) + 2f(x_1) + 2f(x_2) + \cdots + 2f(x_{n-1}) + f(x_n)\right)$$

```
h = (b − a)/n
sum = (f(a) + f(b))/2
for i = 1 to n − 1
    sum = sum + f(x_i)
end
sum = sum · h
```

Accuracy

Look first a basic Trapezoid:

$$\int_a^b f(x)\,dx \approx \frac{1}{2}(b-a)(f(a)+f(b))$$

Looking at the error

$$E = \int_a^b f(x)\,dx - \int_a^b \frac{(b-x)f(a)}{b-a} + \frac{(x-a)f(b)}{b-a}\,dx$$
$$= \int_a^b \frac{(b-a)f(x) - (b-x)f(a) - (x-a)f(b)}{b-a}\,dx$$

Apply change of variable

$$x = a + (b-a)t$$

$$g(t) = f(a + t(b-a))$$

Accuracy

We have changed the interval from $[a, b]$ to $[0, 1]$

$$E = (b-a)\int_0^1 g(t)\,dt - g(0)(b-a)\int_0^1 (1-t)\,dt - g(1)(b-a)\int_0^1 t\,dt$$
$$= (b-a)\left\{\int_0^1 g(t)\,dt - \frac{1}{2}[g(0)+g(1)]\right\}$$

The expression in braces is the error in the trapezoidal rule on the interval $[0, 1]$. Using the expression for the error in linear interpolation on $[0, 1]$

$$g(t) - p(t) = \frac{1}{2}g''(\eta)t(t-1)$$

Integrating and applying the MVT for integrals the expression in braces becomes.

$$\int_0^1 [g(t) - p(t)] = \frac{1}{2}g''(\zeta)\int_0^1 t^2 - t\,dt = -\frac{1}{12}g''(\zeta)$$

Accuracy

Recalling our change of variable the expression for $g''(t)$ is:

$$\begin{aligned} g(t) &= f(a + t(b-a)) \\ g'(t) &= \frac{df}{dx}\frac{dx}{dt} = f'(x)(b-a) \\ g''(t) &= f''(x)(b-a)^2 \end{aligned}$$

using this the expression for the error on $[0,1]$ becomes

$$-\frac{1}{12}g''(\zeta) = -\frac{(b-a)^2}{12}f''(\xi)$$

And the error on $[a,b]$ becomes

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

Accuracy

What about Composite Trapezoid?

$$T(f;P) = \int_a^b f(x)\,dx \approx \frac{h}{2}\sum_{i=0}^{n-1} f(x_i) + f(x_{i+1})$$

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

$$E_i = -\frac{h^3 f''(\eta_i)}{12}$$

So the total error is

$$\begin{aligned}\sum_{i=0}^{n-1} E_i &= \sum_{i=0}^{n-1} -\frac{h^3 f''(\eta_i)}{12} \\ &= -n\frac{h^3 f''(\eta)}{12}(IVT) \\ &= -\frac{(b-a)h^2 f''(\eta)}{12}\end{aligned}$$

Example

How many points should be used to ensure the composite Trapezoid rule is accurate to 10^{-6} for $\int_0^1 e^{-x^2}\,dx$? Need

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

How big is $f''(x)$?

$$\begin{aligned}
f(x) &= e^{-x^2} \\
f'(x) &= -2xe^{-x^2} \\
f''(x) &= -2e^{-x^2} + 4x^2e^{-x^2} \\
f'''(x) &= 12xe^{-x^2} - 8x^3e{-}x^2
\end{aligned}$$

So f''' is always positive. So f'' is monotone increasing and thus take on a maximum at an endpoint: $f''(0) = 2$. Then bound

$$\frac{(b-a)2h^2}{12} \leqslant 10^{-6}$$

Or

$$h^2 \leqslant 6 \times 10^{-6} \quad \Rightarrow \quad \sqrt{(1/6)}10^3 \leqslant n$$

or $n > 410$.

How do we improve Trapezoid?

- instead of a linear approximation, use a quadratic approximation
- $\Rightarrow$ Simpson's Rule

Simpson

- consider $\int_a^b f(x)\,dx$
- partition $P = \{a, a+h, b = a+2h\}$
- or $\int_0^{2h} f(x)\,dx$
- partition $P = \{0, h, 2h\}$
- replace $f(x)$ by a quadratic $p(x)$:

$$
\begin{aligned}
f(x) &\approx p(x) \\
&= f(0) + \frac{f(h) - f(0)}{h} x + \frac{f(2h) - 2f(h) + f(0)}{2h^2} x(x-h) \\
&= \text{newton form}
\end{aligned}
$$

- integrate $\int_0^{2h} p(x)\,dx$:

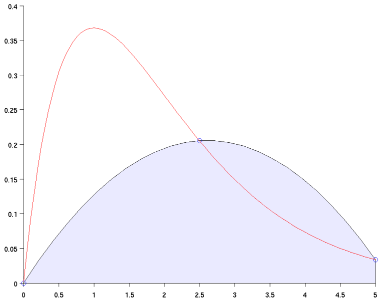
$$
\begin{aligned}
\int_0^{2h} f(x)\,dx &\approx \int_0^{2h} p(x)\,dx \\
&= \frac{h}{3}\left[f(0) + 4f(h) + f(2h)\right]
\end{aligned}
$$

Simpson

Since $b - a = 2h$ we have

basic Simpson's Rule

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



Composite Simpson

Over a uniform partition $P = x_0, x_1, \ldots, x_n$, use Basic Simpson's Rule over each subinterval $[x_{2i}, x_{2i+2}]$

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n/2-1} \int_{x_{2i}}^{x_{2i+2}} f(x)\,dx$$

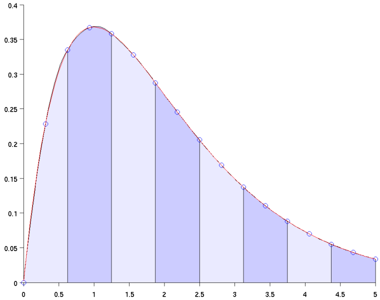
$$= \sum_{i=0}^{n/2-1} \frac{2h}{6}\left[f(x_{2i}) + 4f(x_{2i+1}) + f(x_{2i+2})\right]$$

$$= \frac{h}{3}\left[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots + 4f(x_{n-1}) + f(x_n)\right]$$

Simpson

Composite Simpson's Rule

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



Simpson

How accurate is Simpson? Recall composite Trapezoid:

$$I - T(f, P) = -\frac{1}{12}(b-a)h^2 f''(\xi) - \mathcal{O}(h^2)$$

Prediction? $\mathcal{O}(h^2)$? $\mathcal{O}(h^3)$? $\mathcal{O}(h^4)$?

`int_simpson_test.m`

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

Taylor Series:

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

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

This gives

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

Integrating the Taylor Series expansion of $f(x)$ exactly gives

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

So basic Simpson's Rule gives an error of

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

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

basic Simpson's Rule:

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

Over $n/2$ subintervals $[x_{2i}, x_{2i+2}]$ becomes:

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

Composite Simpson's Rule

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

We "gain" two orders over Trapezoid

Can we generalize?

Summary:

- left/right Riemann: approximate $f(x)$ by 0-degree $p(x)$ and integrate
- Trapezoid: approximate $f(x)$ by 1-degree $p(x)$ and integrate
- Simpson: approximate $f(x)$ by 2-degree $p(x)$ and integrate

Degree of Precision

If the integration rule has zero error when integrating any polynomial of degree $\leqslant r$

and

If the error is nonzero for some polynomial of degree $r+1$,
and

then, the rule has *degree of precision* equal to r.

(basic) Newton-Cotes rules:

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

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	$-\frac{2(b-a)h^6}{945}f^{(6)}(\xi)$	$h=(b-a)/4$