Numerical Differentiation and Integration

Examples of Applications:

- Total quantity of heat or heat transfer $\int\int \; flux \; dA$ (Chemical and Biomedical Engineering)
- Total mass $\sum c_i \Delta V_i \to \int\int\int c(V)dV$ (Chemical and Biomedical Engineering)
- Effective force on a sailboat mast (Civil Engineering)
- Root mean square current (Electrical Engineering)
- Total work (Aerospace and Mechanical Engineering)
- Total amount under any curve (physical, financial, theoretical)
- Find velocity from position data or acceleration from velocity data

An example from Burden and Faires (Epperson example is similar): A sheet of corrugated roofing is constructed using a machine that presses a flat sheet of aluminum into one whose cross-section has the form of a sine wave. A corrugated sheet 4 ft long is needed, the height of the wave is 1 inch from the center line and each wave has a period of 2π inches. Find the length of the flat sheet needed. $L = \int_0^{48} \sqrt{1+\cos^2 x} \; dx$ cannot be integrated easily so we compute it numerically.

Integration smooths. We can always take the derivative of an integral. For example, if $y = x$ on [0,1] and $y = 2 - x$ on [1,2], then y is not differentiable. However, y is continuously integrable. (The integral is $\frac{x^2}{2}$ on [0,1] and $-1 + 2x - \frac{x^2}{2}$ on [1,2]).

Differentiation is easier than integration analytically. It can be performed systematically on many very messy functions. However, differentiation makes a curve more jagged or the derivative might not exist, even when the function is continuous. Computing a derivative numerically is more unstable than integration.

Ways to Derive Differentiation Formulas

Taylor Series and Brute Force

If we write the Taylor Series for $f(x)$ and $f(x+h)$, we can use these to find an approximation for $f'(x)$. We solve for $f'(x)$ giving

$$f'(x) \;=\; \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(\xi)$$

So the error $E \leq \frac{hM}{2}$ where M is biggest f'' can get on the interval.

We can find differentiation formulas using specific points. E.g. Use $f(x), f(x+h)$ and $f(x-h)$ to find an expression for $f''(x)$.

- We begin by writing the Taylor series for $f(x), f(x+h)$ and $f(x-h)$.
- Solve $Af(x+h) \ + \ Bf(x) \ + \ Cf(x-h) \ = \ f''(x) \ +$ with the best error we can get. I.e., we try to eliminate terms with lowest powers of h first.
- This leads to a system of linear equations that can be solved to obtain

$$f''(x) \simeq \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

- Expanding this we find $\dfrac{f(x+h) - 2f(x) + f(x-h)}{h^2} \ = \ f''(x) \ + \ \dfrac{h^2}{12} f''''(\xi).$

Note: we assume that f has as many continuous derivatives as we desire. We need at least 2 points for a first derivative formula, but more points can be used to give better (higher order) error. Reducing h will reduce error further.

Examples:

- Use the Taylor series method (brute force) to find $f'(x_0)$ using x_0 and x_0+h DONE ABOVE
- Use the Taylor series method using $f(x_0+h), f(x_0)$ and $f(x_0-h)$ to find an approximation for $f'(x_0)$ (gives centered difference formula)
- Use the Taylor series method using $f(x_0+h),\ f(x_0)$ and $f(x_0-h)$ to find an approximation for $f''(x_0)$

<u>*Lagrange Polynomial*</u>

We find the Lagrange Polynomial through the grid points and compute the desired derivative from this polynomial.

Example: Use the Lagrange Polynomial through $f(x_0+h),\ f(x_0)$ and $f(x_0-h)$ to find an approximation for $f''(x_0)$.

- $$\begin{aligned} f(x) \quad \simeq \quad L(x) \ = & \\ & \tfrac{(x-x_0)(x-(x_0+h))}{((x_0-h)-x_0)((x_0-h)-(x_0+h))} f(x_0-h) + \tfrac{(x-(x_0-h))(x-(x_0+h))}{(x_0-(x_0-h))(x_0-(x_0+h))} f(x_0) \\ & + \tfrac{(x-(x_0-h))(x-x_0)}{((x_0+h)-(x_0-h))((x_0+h)-x_0)} f(x_0+h) \end{aligned}$$

- Take 2 derivatives to get $f''(x) \simeq \frac{f(x_0+h)-2f(x_0)+f(x_0-h)}{h^2}$.
- We can find the error by taking 2 derivatives of the Lagrange polynomial error $\frac{(x-(x_0-h))(x-x_0)(x-(x_0+h))}{3!} f'''(\xi)$. It can get pretty messy. It is difficult to compute the error this way and we can get incorrect answers since sometimes (as in this case) there is cancellation in the Taylor series analysis that does not appear in the Lagrange analysis.
- Here, the Lagrange analysis gives error $= -h^2 f'''(\xi)/3$. So even if we use this method for finding the approximation formula, it is best to do the analysis for error using the Taylor Series expansion.

Example: Use the Lagrange line from x_0 to x_1 to find a formula for $f'(x_0)$
Example: Use the Lagrange Polynomial through $f(x_0+h)$, $f(x_0)$ and $f(x_0-h)$ to find an approximation for $f'(x_0)$

Using previous results to obtain new formulas

Example:
- Consider the formula we derived for $f'(x_0)$ using $x_0 - h$ and $x_0 + h$.
- Consider this formula for $f'(x_0 + h/2)$ and $f'(x_0 - h/2)$.
- $f'(x_0+h/2) \simeq \frac{f(x_0+h)-f(x_0)}{h}$ and $f'(x_0-h/2) \simeq \frac{f(x_0+h)-f(x_0)}{h}$
- Then $f''(x_0) \simeq \frac{f'(x_0+h/2)-f'(x_0-h/2)}{h}$ yielding
- $$f''(x_0) \simeq \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2}$$

We can find a formula for $f'''(x_0)$ from this second derivative formula using $f''(x_0+h)$ and $f''(x_0-h)$ yielding

$$f'''(x_0) \simeq \frac{f(x_0+2h) - 2f(x_0+h) + 2f(x_0-h) - f(x_0-2h)}{2h^3}$$

Example: Find a 5 point formula for the fourth derivative at x_0 using the second derivative of a second derivatve.
Using $f''(x_0+h)$ and $f''(x_0-h)$ yields $f''''(x_0) \simeq \frac{f(x_0+2h)-4f(x_0+h)+6f(x_0)-4f(x_0-h)+f(x-2h)}{h^4}$.

This method is not as systematic as the others, so it is more limited in scope but it is still pretty neat and easy when it *can* be applied.

Some numerical differentiation formulas:

$$\begin{aligned}
f'(x) &= \tfrac{f(x+h)-f(x)}{h} - \tfrac{h}{2}f''(\xi) \\
f'(x) &= \tfrac{f(x+h)-f(x-h)}{2h} - \tfrac{h^2}{6}f''(\xi) \quad \text{centered difference} \\
f'(x) &= \tfrac{-3f(x)+4f(x+h)-f(x+2h)}{2h} + \tfrac{h^2}{3}f'''(\xi) \\
f''(x) &= \tfrac{f(x+h)-2f(x)+f(x-h)}{h^2} - \tfrac{h^2}{12}f''''(\xi) \quad \text{centered difference} \\
f'''(x_0) &\simeq \tfrac{f(x_0+2h)-2f(x_0+h)+2f(x_0-h)-f(x_0-2h)}{2h^3} \quad \text{centered difference}
\end{aligned}$$

Some Error analysis:

Sometimes taking smaller values of h helps only up to a point. For example, apply $f'(x) \simeq \frac{f(x+h)-f(x)}{h}$. Suppose there is a round-off error of ϵ in computing $f(x)$. Then

$$|f'(x)_{computed} - f'(x)_{exact}| \leq \frac{\epsilon+\epsilon}{h} + \frac{hM}{2}$$

The first term grows as h shrinks. We can find the "best" h by finding the minimum of this error. Thus, $h \simeq 2\sqrt{\frac{\epsilon}{M}}$ is best. For smaller values of h, errors grow.

Another example, apply $f'(x) \simeq \frac{f(x+h)-f(x-h)}{2h}$ with error $\frac{h^2}{6}f'''(\xi)$. So minimize $\frac{\epsilon+\epsilon}{2h} + \frac{h^2 M}{6}$. Again, suppose there is a round-off error of ϵ in computing $f(x)$. Then

$$|f'(x)_{computed} - f'(x)_{exact}| \leq \frac{\epsilon+\epsilon}{2h} + \frac{h^2 M}{6}$$

Minimizing this error gives the best $h \simeq \left(\frac{3\epsilon}{M}\right)^{1/3}$.

Richardson Extrapolation

Let $N(h)$ represent the value of the desired derivative for a step size of h. Write out the Taylor series for step size h and $h/2$ and eliminate the first error term, assuming the derivative based constant (ξ) is the same for both.
E.g., $N(h) = \frac{f(x+h)-f(x)}{h} = f'(x) + \frac{h}{2}f''(x) + \frac{h^2}{6}f'''(x) + \ldots$
$N(h/2) = \frac{f(x+h/2)-f(x)}{h/2} = f'(x) + \frac{h}{4}f''(x) + \frac{h^2}{24}f'''(x) + \ldots$
Thus, an improved estimate of the derivative, $M(h) \equiv 2N(\frac{h}{2}) - N(h) = f'(x) + O(h^2)$.

We can then repeat thus process using $N(h/4)$ to eliminate the h^2 term.
$M(h/2) = 2N(\frac{h}{4}) - N(\frac{h}{2}) = f'(x) + O((h/2)^2)$
So $f'(x) \simeq \frac{4M(h/2)-M(h)}{3}$ with error order h^3.

In general, in order to eliminate h^p terms, use $\frac{2^p M(fine) - M(coarse)}{2^p - 1}$.

We can set up a chart: Suppose $N(h) = f^{(m)}(x) + c_1 h^p + c_2 h^q + c_3 h^r + c_4 h^s + ...$

Error	h^p	h^q	h^r	h^s
	$N(h)$	$\frac{2^p N(h/2) - N(h)}{2^p - 1} = M(h)$	$\frac{2^q M(h/2) - M(h)}{2^q - 1} = L(h)$	$\frac{2^r L(h/2) - L(h)}{2^r - 1}$
	$N(h/2)$	$\frac{2^p N(h/4) - N(h/2)}{2^p - 1} = M(h/2)$	$\frac{2^q M(h/4) - M(h/2)}{2^q - 1} = L(h/2)$	
	$N(h/4)$	$\frac{2^p N(h/8) - N(h/4)}{2^p - 1} = M(h/4)$		
	$N(h/8)$			

Example: Approximate $f'(0)$ for e^x using the centered difference formula

$$f'(x) \simeq \frac{f(x+h) - f(x-h)}{2h} + c_1 h^2 + c_2 h^4 + c_3 h^6 + ...$$

Use $h = 1, 0.5$ and 0.25.

We can find a five point method for $f'(x)$ using Richardson extrapolation with the above formula using h and $2h$. Work it out.

A variation on Richardson Extrapolation

The ratio of grid spacing need not 2:1. We reproduce the table for the case in which the ratio is 3:1.

Error	h^p	h^q	h^r	h^s
	$N(h)$	$\frac{3^p N(h/3) - N(h)}{3^p - 1} = M(h)$	$\frac{3^q M(h/3) - M(h)}{3^q - 1} = L(h)$	$\frac{3^r L(h/3) - L(h)}{3^r - 1}$
	$N(h/3)$	$\frac{3^p N(h/9) - N(h/3)}{3^p - 1} = M(h/3)$	$\frac{3^q M(h/9) - M(h/3)}{3^q - 1} = L(h/3)$	
	$N(h/9)$	$\frac{3^p N(h/27) - N(h/9)}{3^p - 1} = M(h/9)$		
	$N(h/27)$			

If the data points come from experiments, one can fit a Lagrange polynomial or a cubic spline through the points, and take the derivative. Typically, experimental values have some error and performing numerical differentiation on these values is not very stable and amplifies the errors. It is best to fit using low order polynomials or using least squares.

Numerical Integration

We want to approximate the integral of $f(x)$ on [a,b] using function values at some number of grid points.

Trapezoidal Rule:

- Consider the Lagrange polynomial for 2 points x_0 and x_1.
- Then $\int_{x_0}^{x_1} f(x)\ dx \ = \ \int_{x_0}^{x_1}[\frac{x-x_1}{x_0-x_1}f(x_0) + \frac{x-x_0}{x_1-x_0}f(x_1) + \frac{f''(\xi(x))(x-x_0)(x-x_1)}{2}]\ dx$.
- We can pull out the $f''(\xi(x))$ term because the rest doesn't change sign on the interval. Letting $h = x_1 - x_0$ leads to

$$\int_{x_0}^{x_1} f(x)dx \ = \ \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12}f''(\xi)$$

- Using Lagrange polynomials is much more messy as you use higher degree polynomials.

Using Richardson Extrapolation on the Trapezoidal rule gives:

- $\int_{x_0}^{x_2} f(x)dx \ = \ \frac{1}{2}2h[f(x_0) + f(x_2)] + \frac{(2h)^3}{12}f''(\xi_1)$ and
- $\int_{x_0}^{x_2} f(x)dx \ = \ \frac{1}{2}h[f(x_0) + f(x_1)] + \frac{1}{2}h[f(x_1) + f(x_2)] + \frac{h^3}{12}[f''(\xi_3) + f''(\xi_4)]$
- $\qquad = \ \frac{1}{2}h[f(x_0) + 2f(x_1) + f(x_2)] + \frac{h^3}{6}f''(\xi_5)$.
- We eliminate the h^3 terms: $\frac{4fine-1coarse}{3}$ to get

$$\frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] + \text{ higher order terms}$$

- This is called Simpson's Rule. We did not get the error term from this.

We can also derive Simpson's Rule using $\int_{x_1-h}^{x_1+h} f(x)dx =$

$$\begin{aligned}
&\int_{x_1-h}^{x_1+h} f(x_1)+(x-x_1)f'(x_1)+\tfrac{1}{2}(x-x_1)^2f''(x_1)+\tfrac{1}{6}(x-x_1)^3f'''(x_1)+\tfrac{f''''(\xi(x))}{24}(x-x_1)^4dx \\
&= \ xf(x_1) + \tfrac{(x-x_1)^2}{2}f'(x_1) + \tfrac{(x-x_1)^3}{6}f''(x_1) + \tfrac{(x-x_1)^4}{24}f'''(x_1) + \tfrac{(x-x_1)^5}{120}f''''(x_1)\Big|_{x_1-h}^{x_1+h} \\
&= \ 2hf(x_1) + 0 + \tfrac{2h^3}{6}f''(x_1) + 0 + \tfrac{h^5}{60}f''''(\xi_1) \\
&= \ 2hf(x_1) + 0 + \tfrac{h^3}{3}\left(\tfrac{f(x_2)-2f(x_1)+f(x_0)}{h^2} - \tfrac{h^2}{12}f''''(\xi_2)\right) + \tfrac{h^5}{60}f''''(\xi_1) \\
&= \ \tfrac{h}{3}(f(x_2) + 4f(x_1) + f(x_0)) - \tfrac{h^5}{90}f''''(\xi_3)
\end{aligned}$$

One can also derive the Trapezoidal Rule and Simpson's Rule from the Newton-Gregory formulas for approximation of equispaced data points where $dx \ = \ hd\alpha$ and $\alpha \ = \ \frac{x-a}{h}$.

Trapezoidal:

$$\begin{aligned} I &= \int_a^b [f(a) + \Delta f(a)\alpha + \tfrac{f''(\xi)}{2}\alpha(\alpha-1)h^2]dx \\ &= h\int_0^1 [f(a) + \Delta f(a)\alpha + \tfrac{f''(\xi)}{2}\alpha(\alpha-1)h^2]d\alpha \\ &= \tfrac{h}{2}[f(a) + f(b)] - \tfrac{h^3}{12}f''(\xi) \end{aligned}$$

Simpson:

$$\begin{aligned} I &= \int_{x_0}^{x_2} [f(x_0) + \Delta f(x_0)\alpha + \tfrac{\Delta^2 f(x_0)}{2}\alpha(\alpha-1) + \tfrac{\Delta^3 f(x_0)}{6}\alpha(\alpha-1)(\alpha-2) \\ &\quad + \tfrac{f''''(\xi)}{24}\alpha(\alpha-1)(\alpha-2)(\alpha-3)h^4]dx \\ &= h\int_0^2 [f(x_0) + \Delta f(x_0)\alpha + \tfrac{\Delta^2 f(x_0)}{2}\alpha(\alpha-1) + \tfrac{\Delta^3 f(x_0)}{6}\alpha(\alpha-1)(\alpha-2) \\ &\quad + \tfrac{f''''(\xi)}{24}\alpha(\alpha-1)(\alpha-2)(\alpha-3)h^4]d\alpha \\ &= h[2f(x_0) + 2\Delta f(x_0) + \tfrac{\Delta^2 f(x_0)}{3} + 0\Delta^3 f(x_0) - \tfrac{1}{90}f''''(\xi)h^4] \\ &= h[2f(x_0) + 2(f(x_1) - f(x_0)) + \tfrac{f(x_2)-2f(x_1)+f(x_0)}{3} + 0\Delta^3 f(x_0) - \tfrac{1}{90}f''''(\xi)h^4] \\ &= \tfrac{h}{3}[f(x_0) + 4(f(x_1) + f(x_2)] - \tfrac{1}{90}f''''(\xi)h^5] \end{aligned}$$

Midpoint Method or Rectangle Rule

$\int_{x_0}^{x_1} f(x)dx = hf(\frac{x_0+x_1}{2}) +$ Error term. Notice that the function value used is not at the end of the interval. Such a method is called an *Open Newton-Cotes formula.* The Trapezoidal Rule and Simpson's Rule are *Closed Newton-Cotes formulas* since the endpoints are included in the computation. We can compute the error term by finding the lowest degree polynomial for which the method is not exact and get the constant from the error in that term. (This is not a proof, but it works and it makes sense).

Consider $y = 1$ on $[0,h]$ using the Midpoint method
Consider $y = x$ on $[0,h]$ using the Midpoint method
Consider $y = x^2$ on $[0,h]$ using the Midpoint method
The result is that the Midpoint Method approximation = Exact - $\frac{h^3}{12}\frac{f''(\xi)}{2}$.
So the Exact value of the integral is $\int_a^b f(x)dx = (b-a)f(\frac{a+b}{2}) + \frac{h^3}{24}f''(\xi)$

One could also derive all of the above integration formulas by matching coefficients with as many monomials as possible.

- Consider the method $\displaystyle\int_{x_0}^{x_3} f(x) \simeq Af(x_1) + Bf(x_2)$ (i.e. on $[0,3h]$). We are looking for a 2-point Newton-Cotes formula.
- Match for $y = 1$ and $y = x$.
- Note that the integral of $y = x^2$ is not exact with the computed values of A and

B. Relate the error to $f''(x)$.

- Result: $\int_0^{3h} f(x)dx \;=\; \frac{3}{2}h[f(h)+f(2h)] + \frac{3}{4}h^3 f''(\xi)$.

Using Lagrange Polynomials to obtain the coefficients:
Consider the Lagrange polynomial through $x_0, x_1, \ldots, x_n$.
Let l_i be the Lagrange polynomial that is 1 at x_i and 0 at the other xs.
Let $M_i \;=\; \displaystyle\int_{x_0}^{x_n} l_i dx$.
The Lagrange polynomial through $(x_i, f(x_i))$ is $\displaystyle\sum_{i=0}^{n} a_i l_i \;=\; \sum_{i=0}^{n} f(x_i) l_i(x)$.
Thus, $\displaystyle\int_{x_0}^{x_n} f(x)dx \simeq \sum_{i=0}^{n} a_i M_i$.

Example: For x_0, x_1 and x_2 equispaced at $0, h$, and $2h$, we have
$L_0 \;=\; \dfrac{(x-h)(x-2h)}{2h^2}$, $L_1 \;=\; \dfrac{(x)(x-2h)}{-h^2}$, and $L_2 \;=\; \dfrac{(x)(x-h)}{2h^2}$.
Also, $\displaystyle\int_0^{2h} L_0 dx \;=\; \frac{h}{3}$, $\displaystyle\int_0^{2h} L_1 dx \;=\; \frac{4h}{3}$, and $\displaystyle\int_0^{2h} L_2 dx \;=\; \frac{h}{3}$.
So, $\displaystyle\int_{x_0}^{x_2} f(x)dx \simeq \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)]$.
The Lagrange Polynomial technique just described must be exact for polynomials up to degree n since the Lagrange Polynomial is exact for polynomials up to degree n (i.e., given $n+1$ points).

The *degree of precision* of an integration method is the highest power for which the method is exact. I.e., a method with degree of precision n gives exact integrals for all polynomials of degree n or lower.

Newton-Cotes Formula Theorem

CLOSED Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $n+1$ point closed (uses endpoints) Newton-Cotes formula with $x_0 = a$ and $x_n = b$ and $h = \frac{b-a}{n}$. Then $\exists$ a $\xi \in [a,b]$ for which

$$\int_a^b f(x)dx \;=\; \sum_{i=0}^{n} a_i f(x_i) \;+\; h^{n+3}\frac{f^{(n+2)}(\xi)}{(n+2)!}\int_0^n t^2(t-1)\ldots(t-n)dt$$

for n even and $f \in C^{n+2}[a,b]$. There are an odd number of points. We get an extra order (degree of precision) by symmetry.

If n is odd (i.e. an even number of points)

$$\int_a^b f(x)dx \;=\; \sum_{i=0}^{n} a_i f(x_i) \;+\; h^{n+2}\frac{f^{(n+1)}(\xi)}{(n+1)!}\int_0^n t(t-1)\dots(t-n)dt$$

if $f \in C^{n+1}[a,b]$.

Recall that the degree of precision means highest degree monomial integrated exactly.

Number of points	n	Deg. precision	Leading Error Term	Comment
2	1	1	h^3	Trapezoidal
3	2	3	h^5	Simpson's
4	3	3	h^5	Simpson's 3/8 rule

It is most efficient to have an odd number of points.
Some Closed Newton-Cotes formulas are:

2 points: $\int_{x_0}^{x_1} f(x)dx \;=\; \frac{(x_1-x_0)}{2}[f(x_0)+f(x_1)] \;-\; \frac{h^3}{12}f''(\xi)$

3 points: $\int_{x_0}^{x_2} f(x)dx \;=\; \frac{(x_2-x_0)}{6}[f(x_0)+4f(x_1)+f(x_2)] \;-\; \frac{h^5}{90}f^{(4)}(\xi)$

4 points: $\int_{x_0}^{x_3} f(x)dx \;=\; \frac{(x_3-x_0)}{8}[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)] \;-\; \frac{3h^5}{80}f^{(4)}(\xi)$

5 points: $\int_{x_0}^{x_4} f(x)dx \;=\; \frac{(x_4-x_0)}{90}[7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)] - \frac{8h^7}{945}f^{(6)}(\xi)$

OPEN Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $n+1$ point open (doesn't use endpoints) Newton-Cotes formula with $x_{-1}=a$ and $x_{n+1}=b$ and $h=\frac{b-a}{n+2}$. Then $\exists$ a $\xi \in [a,b]$ for which

$$\int_a^b f(x)dx \;=\; \sum_{i=0}^{n} a_i f(x_i) \;+\; h^{n+3}\frac{f^{(n+2)}(\xi)}{(n+2)!}\int_{-1}^{n+1} t^2(t-1)\dots(t-n)dt$$

for n even and $f \in C^{n+2}[a,b]$. There is an odd number of points.

For n odd,

$$\int_a^b f(x)dx \;=\; \sum_{i=0}^{n} a_i f(x_i) \;+\; h^{n+2}\frac{f^{(n+1)}(\xi)}{(n+1)!}\int_{-1}^{n+1} t(t-1)\dots(t-n)dt$$

if $f \in C^{n+1}[a,b]$.

Number of points	n	Deg. accuracy	Leading Error Term	Comment
1	0	1	h^3	Midpoint
2	1	1	h^3	
3	2	3	h^5	

So, again, it is most efficient to have an odd number of points.
Some Open Newton-Cotes formulas are:

$$\begin{aligned}
\text{1 point : } \int_{x_{-1}}^{x_1} f(x)dx \;&=\; (x_1 - x_{-1})[f(x_0)] \;+\; \tfrac{h^3}{3} f''(\xi) \\
\text{2 points: } \int_{x_{-1}}^{x_2} f(x)dx \;&=\; \tfrac{(x_2-x_{-1})}{2}[f(x_0) + f(x_1)] \;+\; \tfrac{3h^3}{4} f''(\xi) \text{ and} \\
\text{3 points: } \int_{x_{-1}}^{x_3} f(x)dx \;&=\; \tfrac{(x_3-x_{-1})}{3}[2f(x_0) - f(x_1) + 2f(x_2)] \;+\; \tfrac{14h^5}{45} f^{(4)}(\xi) \text{ and} \\
\text{4 points: } \int_{x_{-1}}^{x_4} f(x)dx \;&=\; \tfrac{(x_4-x_{-1})}{24}[11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)] \;-\; \tfrac{95h^5}{144} f^{(4)}(\xi)
\end{aligned}$$

If we want to determine the degree of precision of an integration scheme, we can just integrate $1, x, x^2, \ldots$ until the scheme is not exact. The method is good up to degree n if Error($\int P_n(x)\ dx) = 0$ but Error($\int P_{n+1}(x)\ dx) \neq 0$.
Example: Find the degree of precision for the quadrature formula

$$\int_a^b f(x)dx \;=\; \frac{9}{4} h f(x_1) \;+\; \frac{3}{4} h f(x_3)$$

where $a = x_0$, $b = x_3$, $h = \frac{b-a}{3}$ and the mesh is equispaced.

Determining that the method is converging appropriately

The error with the Trapezoidal rule and Midpoint method should be $O(h^2)$, while the error with Simpson's rule should be $O(h^4)$. If we perform the computations with 3 grid spacings $4h$, $2h$, and h, we have (with computed value I and exact value E)

$$\begin{aligned}
E \;-\; I_{4h} \;&\simeq\; C(4h)^p \\
E \;-\; I_{2h} \;&\simeq\; C(2h)^p \\
E \;-\; I_h \;&\simeq\; C(h)^p
\end{aligned}$$

The ratio
$$\frac{I_{4h} - I_{2h}}{I_{2h} - I_h} \;=\; \frac{(I_{4h} - E) + (E - I_{2h})}{(I_{2h} - E) + (E - I_h)} \;\simeq\; \frac{-C(4h)^p + C(2h)^p}{-C(2h)^p + C(h)^p} \;=\; \frac{(2h)^p - (4h)^p}{h^p - (2h)^p} \;=\; 2^p$$
So we can tell just from the iterates (before the method converges, whether the convergence is as it ought to be. The change in the iterates using the Trapezoidal rule should decrease by about a factor of 4 with each iteration.

Composite Integration

To use any of the numerical integration methods on a long interval, just break up the interval into pieces and hook up the pieces.

Simpson's Rule: Recall each step of Simpson's rule integrates over a length of $2h$. If $h = \frac{b-a}{n}$ (and n is even) then
$\int_a^b f(x)dx \simeq \frac{h}{3}[f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \ldots + 2f_{n-2} + 4f_{n-1} + f_n]$

Compute $\int_0^\pi \sin x dx$ using $n = 6$, i.e., $h = \pi/6$. (2.00086 vs. exact = 2).

To compute the error, we just add the error for each piece:
$\frac{n}{2}$ pieces, each with error $\frac{h^5 f''''}{90}$ for a total error of $\frac{nh^5 f''''}{(2)(90)} = \frac{(b-a)f''''h^4}{180}$.
So we lose a power (adding order $\frac{1}{h}$ pieces).
The round-off error is roughly:

$$\frac{h}{3}[\epsilon + 4\epsilon + 2\epsilon + ...] = \frac{b-a}{3n}\epsilon[1 + 4 + 2 + ... + 2 + 4 + 1] = \epsilon(b-a).$$

Trapezoidal's Rule: One step error is $\frac{h^3}{12}f''(\xi)$ If $h = \frac{b-a}{n}$ then
$\int_a^b f(x)\ dx \simeq \frac{h}{2}[f_0 + 2f_1 + 2f_2 + \ldots + 2f_{n-2} + 2f_{n-1} + f_n]$
To compute the error:
n pieces with error each $\frac{h^3 f''}{12}$ for a total error of $\frac{nh^3 f''}{12} = \frac{(b-a)f''h^2}{12}$.
Again, we lose a power.

Midpoint method: One step error is $\frac{h^3}{24}f''(\xi)$.
If $h = \frac{b-a}{n}$ then $\int_a^b f(x)dx \simeq h \sum f(\text{midpoints})$.
To compute the error:
n pieces with error each $\frac{h^3 f''}{24}$ for a total error of $\frac{nh^3 f''}{24} = \frac{(b-a)f''h^2}{24}$. As always, we lose a power.

Summary

Rule	1 − step error	n − step error
Trapezoidal Rule	$\frac{h^3}{12}f''$	$\frac{h^2}{12}(b-a)f''$
Midpoint Method	$\frac{h^3}{24}f''$	$\frac{h^2}{24}(b-a)f''$
Simpson's Rule	$\frac{h^5}{90}f''''$	$\frac{h^4}{180}(b-a)f''''$

Romberg Integration

This is the same thing as Richardson Extrapolation. It is called Richardson Extrapolation when it is used for differentiation methods. It is called Romberg Integration when it is performed for integration methods.

The Composite Trapezoidal Rule has error $\simeq c_1h^2 \ + \ c_2h^4 \ + \ c_3h^6 + ...$ (Thus reducing error when the ratio of step sizes, h, is 2:1 becomes $\frac{4fine-coarse}{3}$, the second round gives $\frac{16fine-coarse}{15}$, and the third round gives $\frac{64fine-coarse}{63}$).

Using 1 big interval, we have:

$$\begin{aligned}
T(H) &= \tfrac{1}{2}(b-a)[f(x_0)+f(x_n)] \\
T(H/2) &= \tfrac{1}{4}(b-a)[f(x_0)+2f(x_{n/2})+f(x_n)] \\
T(H/4) &= \tfrac{1}{8}(b-a)[f(x_0)+2f(x_{n/4})+2f(x_{n/2})+2f(x_{3n/4})+f(x_n)] \\
T(H/8) &= \tfrac{1}{16}(b-a)[f(x_0)+2f(x_{n/8})+2f(x_{n/4})+2f(x_{3n/8})+2f(x_{n/2})+ \\
&\quad 2f(x_{5n/8})+2f(x_{3n/4})+2f(x_{7n/8})+f(x_n)]
\end{aligned}$$

Use the first two lines, H and $H/2$, to eliminate the h^2 term and arrive at Simpson's Rule. Use the first 3 lines to eliminate the h^4 term, and so on.

Adaptive Quadrature

If the function to be integrated has relatively constant regions, as well as very volatile regions, we might want to use different step sizes, h, in different regions, to be both efficient and accurate. One technique is to use spacing h on each sub-region and then use step size $h/2$. On regions where the answer differs by more than the tolerance, break into smaller sub-regions, using $h/4$, and continue until solutions on each region change by less than the tolerance when halving h.

Another way to do this is to note that when halving the step size using Simpson's

Rule, the error with the finer grid should be about one-sixteenth the error with the coarse grid. Thus, if the difference between the two Simpson's Rule outcomes on a subinterval is less than 15ϵ where ϵ is the tolerance for error on the subinterval, the finer value may be accepted with some confidence that the error of this finer (halved) computation is less than ϵ.

Gaussian Quadrature

Question: How good of a quadrature formula can you get if you let both the coefficients *and* the x_is vary?

For example, consider the quadrature method:

$$\int_{-1}^{1} f(x)dx \simeq c_0 f(x_0) \ + \ c_1 f(x_1)$$

There are 4 unknowns we need to compute, so we try to match the integrals of $f(x) = 1, x, x^2$ and x^3.
Nonlinear equations arise (write them out). But they can be solved and we find:
$\int_{-1}^{1} f(x)dx \simeq 1 \ f(-\sqrt{3}/3) \ + \ 1 \ f(\sqrt{3}/3)$.

If we want to derive a 3 point method, we can find

$$\int_{-1}^{1} f(x)dx \ \simeq \ \frac{5}{9}f(-.7745) + \frac{8}{9}f(0) + \frac{5}{9}f(.7745)$$

However, these cannot be solved for easily, due to the nonlinearity of the equations that arise from the matching.

This method would be very difficult, or impossible, to apply for more points. In general $c_0, \ldots, c_n$ and $x_0, \ldots, x_n$ once found, should be good up to $\int x^{2n+1}dx$. I.e., the degree of precision is $2n+1$. To find the values, the x_is and c_is, in an easier way involves learning about orthogonal polynomials. For the case we just considered, Legendre polynomials are relevant.

To apply the method to an integral over the region $[a, b]$:

- Transform the interval linearly such that $x = a \to y = -1$ and $x = b \to y = 1$.
- Let $g(y) \ = \ f(a + \frac{b-a}{2}(y+1))$ so that $\int_a^b f(x)dx \ = \ \int_{-1}^{1} g(y)\frac{b-a}{2}dy$.

Thus, once we find the quadrature coefficients (cs) and values of x, we do not have to repeat the procedure for different intervals. We just transform the function and use the same values for the cs and xs.

The error term using Gaussian quadrature with the Legendre points is

$$\frac{2^{2n+3}(n+1)!^4 f^{(2n+2)}(\xi)}{(2n+3)(2n+2)!^3}$$

for the interval from -1 to 1.

An example for which this method does not work well is $\int_{-3}^{3} \frac{2}{1+2x^2}\ dx$.

Experimental Data
In this case, you cannot choose which grid points to use. If the grid points are not equally spaced you can either use piecewise Trapzoidal Rule or try fitting a low degree Lagrange polynomial to the data and integrate the polynomial.

Improper Integrals

Sometimes, we would like to integrate a function out to very large values of x. On the other hand, we might want to integrate a function that blows up for a finite value of x but might still have finite area under it. One well-known and well-studied example is the cumulative normal distribution

$$\int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx$$

For integrals out to $x \to \infty$, we can transform, letting $t = \frac{1}{x}$.
Then $dt = \frac{-1}{x^2} dx$.
The integral $\int_a^\infty f(x)dx \ \rightarrow \ \int_{1/a}^0 f(1/t)(-x^2)dt \ = \ \int_{1/a}^0 f(1/t)\frac{1}{t^2}dt$.

Example: Set up $\displaystyle\int_1^\infty \frac{dx}{x^2+9}$ using this technique.

Of course, if $x = 0$ is in the interval of integration, we need to break the integral into pieces, say $\int_{-a}^{b} f(x)dx$ and then transform the $\int_b^\infty f(x)dx$ as just explained.

For integrals of functions that become infinite at an endpoint, one may apply an Open Newton-Cotes formula to avoid blow-up.

Multiple Integration

Consider $\int\int f(x,y)dxdy$: Just break the problem up into one-dimensional problems, say, across y for various values of x (arriving at a number of integrals $\int f(x_i, y)dy$ values. Then integrate (once) in x. It's easy to make Trapezoidal and Simpson's Rule solvers for multiple dimensions.