Overview

Difference Formulae

The Taylor expansion of continuous and differentiable function of single variable, $f(x)$, around the point $x+h$, is given by,

$$
\begin{aligned}
f(x+h) &= f(x) + hf'(x) + \frac{1}{2!}h^2 f''(x) + \frac{1}{3!}h^3 f'''(x) + \dots \\
&= \sum_{n=0}^{\infty} \frac{h^n}{n!} f^{(n)}(x)
\end{aligned}
$$

Difference Formulae

We can truncate a Taylor expansion to arrive at approximations of different orders,

$$f(x+h) = f(x) + \mathcal{O}(h)$$
$$f(x+h) = f(x) + hf'(x) + \mathcal{O}\left(h^2\right)$$
$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right)$$
$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \frac{1}{6}h^3 f'''(x) + \mathcal{O}\left(h^4\right)$$

The approximations converge to the correct answer as $h \to 0$.

Difference Formulae

Rearranging the first-order approximation yields a first-order approximation to the derivative,

$$f\left(x+h\right)=f\left(x\right)+hf'\left(x\right)+\mathcal{O}\left(h^2\right)$$

Difference Formulae

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$$f\left(x+h\right) = f\left(x\right) + hf'\left(x\right) + \mathcal{O}\left(h^2\right)$$

$$hf'\left(x\right) = f\left(x+h\right) - f\left(x\right) + \mathcal{O}\left(h^2\right)$$

Difference Formulae

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$$f\left(x+h\right)=f\left(x\right)+hf'\left(x\right)+\mathcal{O}\left(h^2\right)$$

$$\boxed{f'\left(x\right)=\frac{f\left(x+h\right)-f\left(x\right)}{h}+\mathcal{O}\left(h\right)} \tag{1}$$

FIRST FORWARD DIFFERENCES

Difference Formulae

Expanding $f\left(x-h\right)$ instead, we get a different approximation with the same error characteristics,

$$f\left(x-h\right)=f\left(x\right)-hf'\left(x\right)+\mathcal{O}\left(h^2\right)$$

Difference Formulae

Expanding $f(x-h)$ instead, we get a different approximation with the same error characteristics,

$$f(x-h) = f(x) - hf'(x) + \mathcal{O}\left(h^2\right)$$

$$hf'(x) = f(x) - f(x-h) + \mathcal{O}\left(h^2\right)$$

Difference Formulae

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$$f\left(x-h\right)=f\left(x\right)-hf'\left(x\right)+\mathcal{O}\left(h^2\right)$$

$$\boxed{f'\left(x\right)=\frac{f\left(x\right)-f\left(x-h\right)}{h}+\mathcal{O}\left(h\right)} \tag{2}$$

FIRST BACKWARD DIFFERENCES

Difference Formulae

We can eliminate higher-order derivatives and get higher-order approximations by taking linear combinations of approximations at different points, giving us a second-order approximation to the derivative,

$$
\begin{aligned}
f(x+h) &= f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right) \\
f(x-h) &= f(x) - hf'(x) + \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right)
\end{aligned}
$$

Difference Formulae

We can eliminate higher-order derivatives and get higher-order approximations by taking linear combinations of approximations at different points, giving us a second-order approximation to the derivative,

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right)$$
$$f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right)$$

$$\begin{aligned} f(x+h) - f(x-h) = {} & +f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \\ & - f(x) + hf'(x) - \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right) \end{aligned}$$

Difference Formulae

We can eliminate higher-order derivatives and get higher-order approximations by taking linear combinations of approximations at different points, giving us a second-order approximation to the derivative,

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right)$$
$$f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right)$$

$$f(x+h) - f(x-h) = 2hf'(x) + \mathcal{O}\left(h^3\right)$$

Difference Formulae

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$$f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right)$$

$$\boxed{f'(x) = \frac{f(x+h) - f(x-h)}{2h} + \mathcal{O}\left(h^2\right)} \tag{3}$$

FIRST CENTRAL DIFFERENCES

Difference Formulae

We can eliminate higher-order derivatives and get higher-order approximations by taking linear combinations of approximations at different points, giving us a second-order approximation to the derivative,

$$f\left(x+h\right) = f\left(x\right) + hf'\left(x\right) + \frac{1}{2}h^2 f''\left(x\right) + \mathcal{O}\left(h^3\right)$$
$$f\left(x-h\right) = f\left(x\right) - hf'\left(x\right) + \frac{1}{2}h^2 f''\left(x\right) + \mathcal{O}\left(h^3\right)$$

$$\boxed{f'\left(x\right) = \frac{f\left(x+h\right) - f\left(x-h\right)}{2h} + \mathcal{O}\left(h^2\right)} \qquad (3)$$

FIRST CENTRAL DIFFERENCES

Not only do the zeroth and second order terms of the Taylor series cancel, ALL other even order terms also cancel.

First central differences converges to the true value of $f'\left(x\right)$ faster than first forward or first backward differences.

Comparison of Forward, Backward, and Central Differences

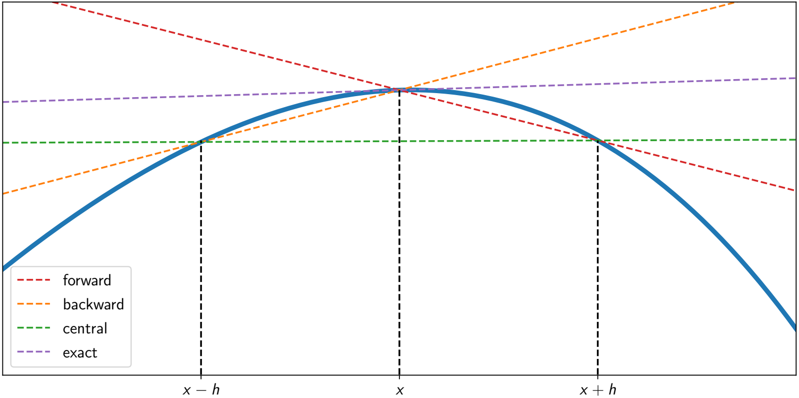

Figure 1: Comparison of the first forward, backward, and central differences methods for $f(x) = x - x^2 + x^3 - x^4$ centred at the point $x = 0.6$ with step size $h = 0.1$.

	forward	backward	central	exact
$f'(0.6)$	-0.135	0.139	0.002	0.016

Table 1: $f'(0.6)$ at several levels of approximation.

Higher order derivatives can also be obtained in this way,

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right)$$
$$f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right)$$

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$$f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right)$$

$$\begin{aligned} f(x+h) + f(x-h) = &+ f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \\ &+ f(x) - hf'(x) + \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right) \end{aligned}$$

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$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + \mathcal{O}(h^3)$$

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$$f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right)$$

$$\boxed{f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}\left(h^2\right)} \tag{4}$$

SECOND CENTRAL DIFFERENCES

We can construct approximations to arbitrary order by adding more and more combinations, *e.g.*, this fourth-order approximation to the first derivative,

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \frac{1}{6}h^3 f'''(x) + \frac{1}{24}h^4 f'''(x) + \mathcal{O}\left(h^5\right)$$
$$f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2 f''(x) - \frac{1}{6}h^3 f'''(x) + \frac{1}{24}h^4 f'''(x) + \mathcal{O}\left(h^5\right)$$
$$f(x+2h) = f(x) + 2hf'(x) + 2h^2 f''(x) + \frac{4}{3}h^3 f'''(x) + \frac{2}{3}h^4 f'''(x) + \mathcal{O}\left(h^5\right)$$
$$f(x-2h) = f(x) - 2hf'(x) + 2h^2 f''(x) - \frac{4}{3}h^3 f'''(x) + \frac{2}{3}h^4 f'''(x) + \mathcal{O}\left(h^5\right)$$

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$$f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2 f''(x) - \frac{1}{6}h^3 f'''(x) + \frac{1}{24}h^4 f''''(x) + \mathcal{O}\left(h^5\right)$$

$$f(x+2h) = f(x) + 2hf'(x) + 2h^2 f''(x) + \frac{4}{3}h^3 f'''(x) + \frac{2}{3}h^4 f''''(x) + \mathcal{O}\left(h^5\right)$$

$$f(x-2h) = f(x) - 2hf'(x) + 2h^2 f''(x) - \frac{4}{3}h^3 f'''(x) + \frac{2}{3}h^4 f''''(x) + \mathcal{O}\left(h^5\right)$$

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{1}{3}h^3 f'''(x) + \mathcal{O}\left(h^5\right)$$

$$f(x+2h) - f(x-2h) = 4hf'(x) + \frac{8}{3}h^3 f'''(x) + \mathcal{O}\left(h^5\right)$$

We can construct approximations to arbitrary order by adding more and more combinations, *e.g.*, this fourth-order approximation to the first derivative,

$$f\left(x+h\right)=f\left(x\right)+hf'\left(x\right)+\frac{1}{2}h^{2}f''\left(x\right)+\frac{1}{6}h^{3}f'''\left(x\right)+\frac{1}{24}h^{4}f'''\left(x\right)+\mathcal{O}\left(h^{5}\right)$$
$$f\left(x-h\right)=f\left(x\right)-hf'\left(x\right)+\frac{1}{2}h^{2}f''\left(x\right)-\frac{1}{6}h^{3}f'''\left(x\right)+\frac{1}{24}h^{4}f'''\left(x\right)+\mathcal{O}\left(h^{5}\right)$$
$$f\left(x+2h\right)=f\left(x\right)+2hf'\left(x\right)+2h^{2}f''\left(x\right)+\frac{4}{3}h^{3}f'''\left(x\right)+\frac{2}{3}h^{4}f'''\left(x\right)+\mathcal{O}\left(h^{5}\right)$$
$$f\left(x-2h\right)=f\left(x\right)-2hf'\left(x\right)+2h^{2}f''\left(x\right)-\frac{4}{3}h^{3}f'''\left(x\right)+\frac{2}{3}h^{4}f'''\left(x\right)+\mathcal{O}\left(h^{5}\right)$$

$$8(f\left(x+h\right)-f\left(x-h\right))-(f\left(x+2h\right)-f\left(x-2h\right))=12hf'\left(x\right)+\mathcal{O}\left(h^{5}\right)$$

We can construct approximations to arbitrary order by adding more and more combinations, *e.g.*, this fourth-order approximation to the first derivative,

$$f\left(x+h\right)=f\left(x\right)+hf'\left(x\right)+\frac{1}{2}h^{2}f''\left(x\right)+\frac{1}{6}h^{3}f'''\left(x\right)+\frac{1}{24}h^{4}f'''\left(x\right)+\mathcal{O}\left(h^{5}\right)$$

$$f\left(x-h\right)=f\left(x\right)-hf'\left(x\right)+\frac{1}{2}h^{2}f''\left(x\right)-\frac{1}{6}h^{3}f'''\left(x\right)+\frac{1}{24}h^{4}f'''\left(x\right)+\mathcal{O}\left(h^{5}\right)$$

$$f\left(x+2h\right)=f\left(x\right)+2hf'\left(x\right)+2h^{2}f''\left(x\right)+\frac{4}{3}h^{3}f'''\left(x\right)+\frac{2}{3}h^{4}f'''\left(x\right)+\mathcal{O}\left(h^{5}\right)$$

$$f\left(x-2h\right)=f\left(x\right)-2hf'\left(x\right)+2h^{2}f''\left(x\right)-\frac{4}{3}h^{3}f'''\left(x\right)+\frac{2}{3}h^{4}f'''\left(x\right)+\mathcal{O}\left(h^{5}\right)$$

$$\boxed{f'\left(x\right)=\frac{f\left(x-2h\right)-8f\left(x-h\right)+8f\left(x+h\right)-f\left(x+2h\right)}{12h}+\mathcal{O}\left(h^{4}\right)} \qquad (5)$$

FIVE POINT FORMULA

Boundaries

A solution for boundary points with the same error order as first central differences can be obtained by taking differences of $f(x+h)\,, f(x+2h)$,

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \mathcal{O}\left(h^3\right)$$
$$f(x+2h) = f(x) + 2hf'(x) + 2h^2 f''(x) + \mathcal{O}\left(h^3\right)$$

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$$f(x+2h) = f(x) + 2hf'(x) + 2h^2 f''(x) + \mathcal{O}\left(h^3\right)$$

$$f(x+2h) - 4f(x+h) = -3f(x) - 2hf'(x) + \mathcal{O}\left(h^3\right)$$

Boundaries

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$$f\left(x+h\right) = f\left(x\right) + hf'\left(x\right) + \frac{1}{2}h^2 f''\left(x\right) + \mathcal{O}\left(h^3\right)$$
$$f\left(x+2h\right) = f\left(x\right) + 2hf'\left(x\right) + 2h^2 f''\left(x\right) + \mathcal{O}\left(h^3\right)$$

$$\boxed{f'\left(x\right) = \frac{4f\left(x+h\right) - 3f\left(x\right) - f\left(x+2h\right)}{2h} + \mathcal{O}\left(h^2\right)} \tag{6}$$

which expression approximates the derivative at x using only x and points to the right of x.

Non-uniform grids

It is easy enough to modify the second central difference equations to incorporate non-uniform spacings a, b,

$$b^2 f(x+a) = b^2 f(x) + ab^2 f'(x) + \frac{1}{2} a^2 b^2 f''(x) + a^3 b^2 f'''(x) + \mathcal{O}\left(a^4\right)$$
$$a^2 f(x-b) = a^2 f(x) - ba^2 f'(x) + \frac{1}{2} b^2 a^2 f''(x) - b^3 a^2 f'''(x) + \mathcal{O}\left(b^4\right),$$

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rearranging,

$$\boxed{f'(x) = \frac{b^2 f(x+a) - a^2 f(x-b) + \left(b^2 - a^2\right) f(x)}{ab(b+a)} + \mathcal{O}\left(h^2\right)} \tag{7}$$

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rearranging,

$$\boxed{f'(x) = \frac{b^2 f(x+a) - a^2 f(x-b) + \left(b^2 - a^2\right) f(x)}{ab(b+a)} + \mathcal{O}\left(h^2\right)} \qquad (7)$$

Notice that, with uneven spacings, only the second order terms in the Taylor series cancel—other, higher-order even terms remain.

Say we can express a problem in the form,

$$A = A(h) + Kh^k + K'h^{k+1} + K''h^{k+2} + \ldots$$

where $h, k, A(h)$ are known, and the constants K^n are in general not known.

Richardson Extrapolation

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Truncating at kth order in h, we get,

$$A = A(h) + Kh^k + \mathcal{O}\left(h^{k+1}\right).$$

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How can we improve the error characteristics of this expression?

Richardson Extrapolation

Once again, we take linear combinations to eliminate the lowest-order unknown term,

$$A = A(h) + Kh^k + \mathcal{O}\left(h^{k+1}\right)$$

$$A = A\left(\frac{h}{2}\right) + K\left(\frac{h}{2}\right)^k + \mathcal{O}\left(h^{k+1}\right)$$

Richardson Extrapolation

Once again, we take linear combinations to eliminate the lowest-order unknown term,

$$A = A\left(h\right) + Kh^{k} + \mathcal{O}\left(h^{k+1}\right)$$

$$A = A\left(\frac{h}{2}\right) + \frac{1}{2^{k}}K\left(h\right)^{k} + \mathcal{O}\left(h^{k+1}\right)$$

Richardson Extrapolation

Once again, we take linear combinations to eliminate the lowest-order unknown term,

$$A = A(h) + Kh^k + \mathcal{O}\left(h^{k+1}\right)$$

$$2^k A = 2^k A\left(\frac{h}{2}\right) + K(h)^k + \mathcal{O}\left(h^{k+1}\right)$$

Richardson Extrapolation

Once again, we take linear combinations to eliminate the lowest-order unknown term,

$$A = A(h) + Kh^k + \mathcal{O}\left(h^{k+1}\right)$$

$$\left(2^k - 1\right) A = 2^k A\left(\frac{h}{2}\right) - A(h) + K(h)^k - K(h)^k + \mathcal{O}\left(h^{k+1}\right)$$

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Once again, we take linear combinations to eliminate the lowest-order unknown term,

$$A = A(h) + Kh^k + \mathcal{O}\left(h^{k+1}\right)$$

$$A = \frac{2^k A\left(\frac{h}{2}\right) - A(h)}{2^k - 1} + \mathcal{O}\left(h^{k+1}\right)$$

Once again, we take linear combinations to eliminate the lowest-order unknown term,

$$A = A(h) + Kh^k + \mathcal{O}\left(h^{k+1}\right)$$

$$\boxed{\begin{aligned} A &= B(h) + \mathcal{O}\left(h^{k+1}\right) \qquad (8) \\ B(h) &= \frac{2^k A\left(\frac{h}{2}\right) - A(h)}{2^k - 1} \qquad (9) \end{aligned}}$$

RICHARDSON EXTRAPOLATION

Richardson Extrapolation: Example

$$\boxed{\begin{aligned} A &= B\left(h\right) + \mathcal{O}\left(h^{k+1}\right) \\ B\left(h\right) &= \frac{2^k A\left(\frac{h}{2}\right) - A\left(h\right)}{2^k - 1} \end{aligned}}$$

let

$$A(h) = \frac{f\left(x+h\right) - f\left(x\right)}{h} + \mathcal{O}\left(h\right)$$

Richardson Extrapolation: Example

$$\boxed{\begin{aligned} A &= B\left(h\right) + \mathcal{O}\left(h^{k+1}\right) \\ B\left(h\right) &= \frac{2^k A\left(\frac{h}{2}\right) - A\left(h\right)}{2^k - 1} \end{aligned}}$$

let

$$A(h) = \frac{f\left(x+h\right) - f\left(x\right)}{h} + \mathcal{O}\left(h\right)$$

then $k = 1$ and

$$B(h) = 2A\left(\frac{h}{2}\right) - A\left(h\right)$$

Richardson Extrapolation: Example

$$\boxed{\begin{aligned} A &= B\left(h\right) + \mathcal{O}\left(h^{k+1}\right) \\ B\left(h\right) &= \frac{2^k A\left(\frac{h}{2}\right) - A\left(h\right)}{2^k - 1} \end{aligned}}$$

let

$$A(h) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}\left(h\right)$$

substituting,

$$B\left(h\right) = 2\frac{f(x+h/2) - f(x)}{\frac{h}{2}} - \frac{f(x+h) - f(x)}{h}$$

Richardson Extrapolation: Example

$$\boxed{\begin{aligned} A &= B\left(h\right) + \mathcal{O}\left(h^{k+1}\right) \\ B\left(h\right) &= \frac{2^k A\left(\frac{h}{2}\right) - A\left(h\right)}{2^k - 1} \end{aligned}}$$

let

$$A(h) = \frac{f\left(x+h\right) - f\left(x\right)}{h} + \mathcal{O}\left(h\right)$$

rearranging,

$$B\left(h\right) = \frac{4f\left(x+h/2\right) - 3f\left(x\right) - f\left(x+h\right)}{h}$$

Richardson Extrapolation: Example

$$\boxed{\begin{aligned} A &= B\left(h\right) + \mathcal{O}\left(h^{k+1}\right) \\ B\left(h\right) &= \frac{2^k A\left(\frac{h}{2}\right) - A\left(h\right)}{2^k - 1} \end{aligned}}$$

let

$$A(h) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}\left(h\right)$$

setting $h \to 2h$,

$$B\left(2h\right) = \frac{4f\left(x+h\right) - 3f\left(x\right) - f\left(x+2h\right)}{2h}$$

which you should remember from equation 6.

Catastrophic Cancellation

All of the difference methods suffer from catastrophic cancellation.

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h)$$

Catastrophic Cancellation

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On a computer, the effective value of h in the expression $x - h$ is not the same as the h in the denominator.

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Remember, float addition is NOT associative, so the parentheses are meaningful.

Complex Differences

We can avoid this problem by taking an imaginary step,

$$f\left(x+ih\right)=f\left(x\right)+ihf'\left(x\right)-\frac{h^2}{2}f''\left(x\right)-i\frac{h^3}{6}f'''\left(x\right)+\mathcal{O}\left(h^4\right)$$

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FIRST COMPLEX DIFFERENCES

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FIRST COMPLEX DIFFERENCES

Addition of a real and imaginary float does not incur precision loss!

Overview

Numerical Integration

A wealth of methods exist for approximating integrals with no closed form (or any other integral, for that matter).

$$\int_a^b \sqrt{1 - x^4}\, dx \qquad \int_a^b \exp\left(-x^2\right) dx$$

$$\int_a^b \frac{1}{log x}\, dx \qquad \int_a^b \frac{\sin x}{x}\, dx$$

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We will look at two classes of approximations,

NEWTON-COTES and GAUSSIAN QUADRATURE

which both work by cutting up the integral into slices,

$$\int_a^b f(x)\,dx = \int_a^{a+h} f(x)\,dx + \ldots + \int_{b-h}^b f(x)\,dx$$

small intervals on which f varies smoothly.

From Taylor series

Idea: integrate a Taylor expansion, then truncate the integral.

$$\int_a^b f(x)\, dx = \int_{-h}^{h} f(x_0 + y)\, dy$$

where $h = (a - b)/2$, $x_0 = (a + b)/2$.

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$$\int_{-h}^{h} f(x_0 + y)\,dy = \int_{-h}^{h} \sum_{n=0}^{\infty} \frac{f^n(x_0)}{n!} y^n$$

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$$= \sum_{n=0}^{\infty} \frac{f^n(x_0)}{n!} \left[\frac{y^{n+1}}{n+1}\right]_{-h}^{h} \tag{12}$$

$$= \sum_{n=0}^{\infty} \frac{f^n(x_0)}{(n+1)!} \left(h^{n+1} - (-h)^{n+1}\right) \tag{13}$$

$$= \sum_{n=0}^{\infty} \frac{f^{2n}(x_0)}{(2n+1)!} 2h^{n+1} \tag{14}$$

First order

$$\boxed{\int_{-h}^{h} f\left(x_0 + y\right) dy = \sum_{n=0}^{\infty} \frac{f^{2n}(x_0)}{(2n+1)!} 2h^{n+1}}$$

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$$\boxed{\begin{gathered}\int_{a}^{b} f\left(x\right) dx \approx 2hf\left(\frac{a+b}{2}\right) \\ h = (a-b)/2\end{gathered}} \tag{15}$$

MIDPOINT RULE

Second order

$$\boxed{\int_{-h}^{h} f\left(x_0 + y\right) dy = \sum_{n=0}^{\infty} \frac{f^{2n}(x_0)}{(2n+1)!} 2h^{n+1}}$$

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Expanding to second order,

$$\int_{-h}^{h} f\left(x_0 + y\right) dy = 2hf(x_0) + \frac{f''(x_0)}{3} h^3 + \mathcal{O}(h^5)$$

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$$\boxed{\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \quad h = (a-b)/2} \tag{16}$$

SIMPSON'S RULE

Summing up: composite rules

- The midpoint rule and Simpson's rule allow us to approximate the integral over a single interval.

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- The approximation improves as the interval becomes smaller (proportional to h^3 for the midpoint rule, h^5 for Simpsons' rule).
- We can take higher-order expansions to get formulae with better asymptotic errors...
- ...or sum up the approximations for many intervals to get smaller errors for each small interval.

Summing up: composite rules

Take the midpoint rule as an example. If the approximation is made as a sum over many intervals,

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n-1}\left[2hf(a+ih) + \mathcal{O}(h^3)\right]; \quad h = \frac{b-a}{2n}$$

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COMPOSITE MIDPOINT RULE

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COMPOSITE MIDPOINT RULE

Notice the leading error term goes down one order of h.

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- Q. How do we choose the weights?
- A. Choose the weights so that integrals of polynomials up to a given order are exact.
- Q. Why is that appealing?
- A. The Taylor expansion of a function about a point is an infinite order polynomial; close to the point, the function and its integral are approximated well by a few low-order monomials.

Deriving Newton-Cotes Weights

For m evenly-spaced points, we get exact results for order-(n-1) polynomials by solving m equations:

$$
\begin{aligned}
f(x) = 1 &\implies \int_{x_1}^{x_m} 1 dx &= x_m - x_1 &= \sum_{i=1}^{m} w_i \cdot 1; \\
f(x) = x &\implies \int_{x_1}^{x_m} x dx &= \frac{1}{2}\left(x_m^2 - x_1^2\right) &= \sum_{i=1}^{m} w_i x_i; \\
\vdots & & & \vdots \\
f(x) = x^{m-1} &\implies \int_{x_1}^{x_m} x^{m-1} dx &= \frac{1}{m}\left(x_m^m - x_1^m\right) &= \sum_{i=1}^{m} w_i x_i^{m-1}.
\end{aligned}
$$

Deriving Newton-Cotes Weights

Solving for a single weight,

$$x_2 - x_1 = \sum_{i=1}^{m=1} w_i f_i$$

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$$\boxed{\begin{array}{c} \int_{x_1}^{x_2} f(x)\,dx \approx hf_1 \\ h = x_2 - x_1 \end{array}} \tag{18}$$

RECTANGLE RULE

Deriving Newton-Cotes Weights

Solving for two weights,

$$x_2 - x_1 = w_1 \cdot 1 + w_2 \cdot 1$$
$$\frac{1}{2}\left(x_2^2 - x_1^2\right) = w_1 x_1 + w_2 x_2$$

by symmetry,

Deriving Newton-Cotes Weights

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$$\implies 2w_1 = x_2 - x_1$$

Deriving Newton-Cotes Weights

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$$\boxed{\begin{gathered}\int_{x_1}^{x_2} f\left(x\right) dx \approx \frac{h}{2}\left(f_1 + f_2\right) \\ h = x_2 - x_1\end{gathered}} \tag{19}$$

TRAPEZIUM RULE

Solving for three weights,

$$\begin{aligned} x_3 - x_1 &= w_1 \cdot 1 + w_2 \cdot 1 + w_3 \cdot 1 \\ \frac{1}{2}\left(x_3^2 - x_1^2\right) &= w_1 x_1 + w_2 x_2 + w_3 x_3 \\ \frac{1}{3}\left(x_3^3 - x_1^3\right) &= w_1 x_1^2 + w_2 x_2^2 + w_3 x_3^2 \end{aligned}$$

By symmetry, $w_1 = w_3$; we also require the x_i to be evenly-spaced, so can write $x_1 = x_2 - h; x_3 = x_2 + h$;
Substituting and rearranging,

Deriving Newton-Cotes Weights

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$$2h = 2w_1 + w_2$$
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Deriving Newton-Cotes Weights

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$$\begin{aligned} 2h &= 2w_1 + w_2 \\ 2hx_2 &= 2w_1 x_2 + w_2 x_2 \\ w_1 &= \frac{1}{3}h \end{aligned}$$

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x_3 - x_1 &= w_1 \cdot 1 + w_2 \cdot 1 + w_3 \cdot 1 \\
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By symmetry, $w_1 = w_3$; we also require the x_i to be evenly-spaced, so can write $x_1 = x_2 - h; x_3 = x_2 + h$;
Substituting and rearranging,

$$
\implies w_1 = \frac{1}{3}h = w_3; \quad w_2 = \frac{4}{3}h.
$$

Deriving Newton-Cotes Weights

Solving for three weights,

$$\begin{aligned} x_3 - x_1 &= w_1 \cdot 1 + w_2 \cdot 1 + w_3 \cdot 1 \\ \frac{1}{2}\left(x_3^2 - x_1^2\right) &= w_1 x_1 + w_2 x_2 + w_3 x_3 \\ \frac{1}{3}\left(x_3^3 - x_1^3\right) &= w_1 x_1^2 + w_2 x_2^2 + w_3 x_3^2 \end{aligned}$$

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$$\boxed{\begin{gathered} \int_{x_1}^{x_3} f(x)\, dx \approx \frac{h}{3}\left(f_1 + 4f_2 + f_3\right) \\ 2h = x_3 - x_1 \end{gathered}} \tag{20}$$

SIMPSON'S RULE

Error in the Trapezium Rule

Compare the trapzeium rule,

$$\int_{-h}^{h} f\left(x+y\right) dy \approx h\left[f(x-h)+f(x+h)\right] = A_{\text{est}}$$

with the exact integral,

$$\int_{-h}^{h} f\left(x+y\right) dy = 2hf(x) + \frac{f''(x)}{3}h^3 + \mathcal{O}(h^5) = A_{\text{exact}}$$

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- at high orders, the Newton–Cotes formulae containing large weights of different signs, leading to loss of precision
- the formulae that come from Richardson extrapolation, Romberg's methods, are relatively stable

Gaussian Quadrature

In deriving the weights for the Newton-Cotes formulae, our goal was to make an m-point approximation to the integral

$$\int_{x_1}^{x_m} f(x)\,dx$$

that was exact for order-$(m-1)$ polynomials.

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James Farrell & Jure Dobnikar

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If a change of coordinates that gives these limits is possible, then

GAUSSIAN QUADRATURE

gives an m-point approximation exact for order-$(2m-1)$ polynomials.

Deriving Gaussian Quadrature nodes and weights

For two points, in this context called nodes, x_1, x_2; $x_1 < x_2$ somewhere on the interval $(-1, 1)$, we have four equations with four unknowns,

$$f(x) = 1 \rightarrow A = \int_{-1}^{1} dx = 2 = w_1 + w_2$$

$$f(x) = x \rightarrow A = \int_{-1}^{1} x dx = 0 = w_1 x_1 + w_2 x_2$$

$$f(x) = x^2 \rightarrow A = \int_{-1}^{1} x^2 dx = \frac{2}{3} = w_1 x_1^2 + w_2 x_2^2$$

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Solving, we find,

$$x_2 = -x_1 = \frac{1}{\sqrt{3}}; \quad w_1 = w_2 = 1.$$

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$$\boxed{\int_{-1}^{1} f(x)\, dx \approx f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)} \tag{21}$$

GAUSSIAN QUADRATURE ON TWO NODES

Coordinate transformation

In the general case of limits $[a, b]$, we must first apply the coordinate transformation,

$$t = \frac{b-a}{2}x + \frac{b+a}{2}$$
$$\int_a^b f(t)\,dt = \int_{-1}^{1} f\left(\frac{b-a}{2}x + \frac{b+a}{2}\right)\frac{b-a}{2}dx \tag{22}$$
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The approximate expression for the integral the becomes,

$$\int_a^b f(t)\,dt \approx \frac{b-a}{2}\sum_{i=1}^{n} w_i f\left(\frac{b-a}{2}x_i + \frac{b+a}{2}\right) \tag{23}$$

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- Gaussian quadrature is more accurate with fewer points, incurring less computational effort...
- ...but requires the function to be sampled at specific points, which is generally not possible with experimental data.
- Newton–Cotes methods can be generalised to work with non-uniform data points, making Simpson's method a good choice from integrating experimental data.