Number Crunching - Classical Numerical Analysis

<u>Example</u> In the next assignment, we may want to find the expected price of oil in December, given an assumption that we know its probability density fctn. $p(x)$. That's

$$E\{\text{price}\} = \int_{-\infty}^{\infty} x\, p(x)\, dx$$

or, say, the probability that the price <u>exceeds</u> a given value V

$$\text{prob.}\{\text{price exceeds } V\} = \int_{V}^{\infty} p(x)\, dx$$

If $p(x)$ is something we can't integrate analytically (Freshman calculus), then we must resort to <u>numerical</u> <u>methods</u>.

→ Problem goes back 200 years to the masters, Newton, Gauss, Euler !

<u>References used</u> [Acton 96] "Real Computing Made Real" — lots of wisdom

[Press et al.] "Numerical Recipes"

$\left.\begin{array}{l}\text{[Atkinson 85]}\\ \text{[Ralston \& Rabinowitz 78]}\\ \text{[Acton 70]}\end{array}\right\}$ classical stuff

- Numerical Integration and interpolation are perhaps the two earliest goals of numerical computation.

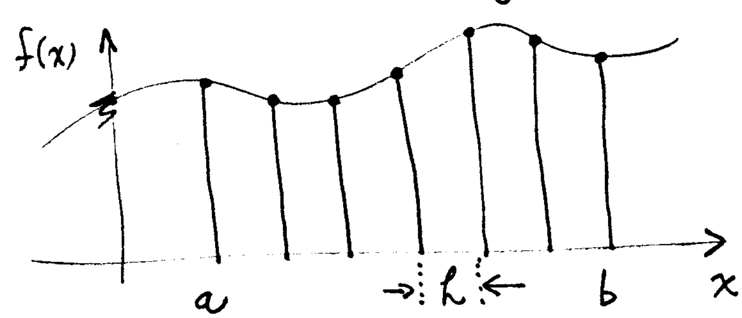
- Generally speaking, Integration is a <u>smoothing</u> operation, & is relatively insensitive to noise, and forgiving.

- interpolation is less forgiving
- differentiation even less forgiving, ... etc.

Our path for the next three assignments is through three central applications of integration:

quadrature ⟶ ode's ⟶ pde's

<u>Strategy for Numerical Integration:</u>



$\int_a^b f(x)dx =$ area under curve $f(x)$

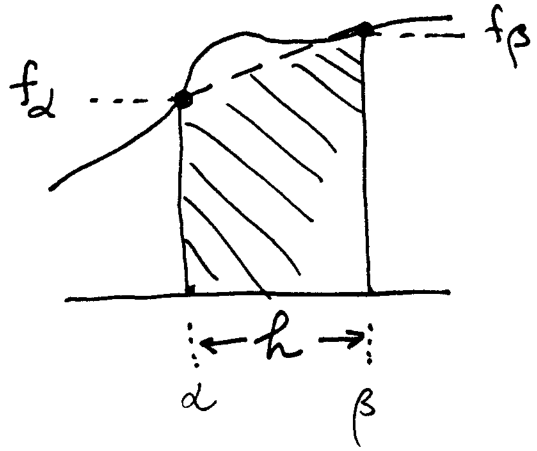
1. Break up interval into pieces of width h

2. Approximate $f(\cdot)$ by a polynomial over a few intervals (degree n, $n+1$ points, n intervals)

3. Integrate these polynomial approximations & add up.

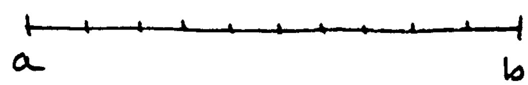
[4. Repeat for smaller h until convergence]

Standard Simple Method: degree 1 polynomials
Trapezoidal Rule
2 points, 1 interval



$$\int_\alpha^\beta f(x)\,dx \approx \text{area under trapezoid} = \frac{h}{2}(f_\alpha + f_\beta)$$

"Extended" Version:

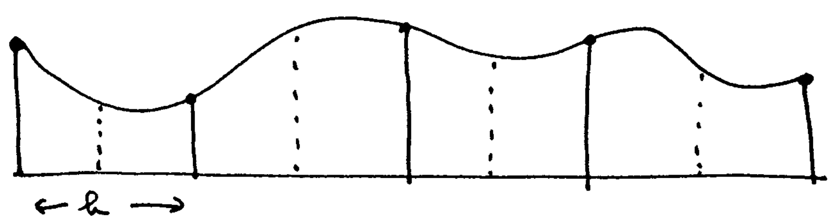


add results for all intervals
$$\left\{\begin{array}{ccccccc} \frac{1}{2} & \frac{1}{2} & & & & & \\ & \frac{1}{2} & \frac{1}{2} & & & & \\ & & \frac{1}{2} & \frac{1}{2} & & \cdots & \end{array}\right.$$

$$h\cdot\left(\tfrac{1}{2}\quad 1\quad 1\quad 1\quad 1\quad \cdots\quad 1\quad \tfrac{1}{2}\right) \leftarrow \text{weights}$$

→ Don't recompute old ordinates when h is halved

[Acton 96]



h $\quad sum_i$ = Solid values, endpoints weighted by 1/2

$h/2$ $\quad sum_{i+1} = sum_i$ + dotted values

↑

save!

Systematic Creep in the abscissae [Acton96]

What's wrong with

$$x_{i+1} = x_i + h \ ?$$

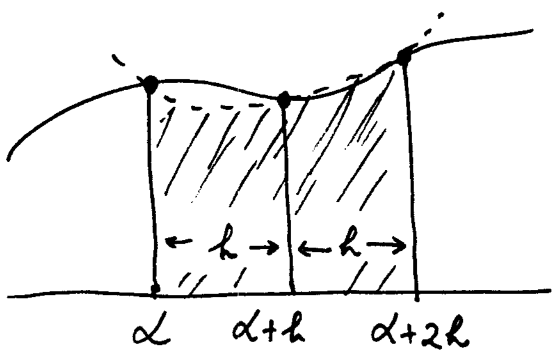
Do

$$x_k = (\text{Interval length}) * k/n \qquad k = 0, \cdots, n$$

Simpson's Rule

the next higher order polynomial

quadratic, 3 points, 2 intervals



$$\int_{\alpha}^{\alpha+2h} f(x)dx \approx \text{area under quadratic}$$

$$= \frac{h}{3}\left[f(\alpha) + 4f(\alpha+h) + f(\alpha+2h) \right]$$

Composite ("extended") Version:

$$\frac{h}{3}\begin{bmatrix} 1 & 4 & 1 & & & & \\ & & 1 & 4 & 1 & & \\ & & & & 1 & 4 & 1 \ \ldots \end{bmatrix}$$

$$\frac{h}{3}\left[\underbrace{1 \ 4 \ 2 \ 4 \ 2 \ 4 \ \cdots \ 4 \ 1}_{\text{Weights}} \right]$$

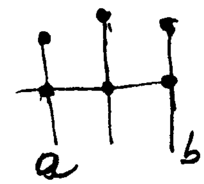
Re-using points in Simpson's Rule is slightly trickier:

$$\frac{3}{h} A_n = 1 \quad 4 \quad 2 \quad 4 \quad 2 \quad 4 \quad \ldots \quad 4 \quad 1$$

$$= \underbrace{1 \ldots 2 \ldots 2 \ldots 2 \ldots 1}_{B_n} + \underbrace{4 \ldots 4 \ldots 4 \ldots 4}_{C_n = 4(\text{sum of new ordinates})}$$

$$\frac{3}{(h/2)} A_{n+1} = \left[B_n + \frac{C_n}{2}\right] + 4 \cdot (\text{sum of new ordinates})$$

Start with $\frac{3}{(b-a)/2} A_1 = \underbrace{1 \ldots 1}_{B_1} + \underbrace{4}_{C_1}$



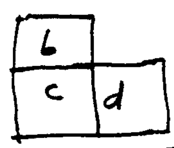
Note that Numerical Recipes [Press et al.] shows how to implement Simpson's Rule using Trapezoidal Rule.
(Eg. 4.2.4, etc)

Additional Refinement of Trapezoidal Rule: Romberg quadratures: [Acton96]

k	0	1	2	3
h	T_{00}			
h/2	T_{01}	R_{11}		
h/4	T_{02}	R_{12}	R_{22}	
h/8	T_{03}	R_{13}	R_{23}	R_{33}
⋮	⋮	⋮		

computed from T's

Trapezoidal Rule approximants

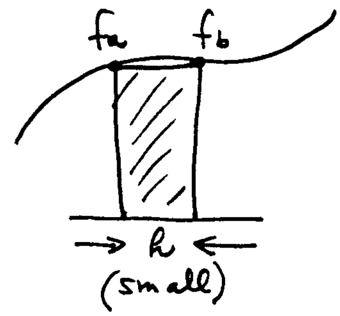


$$d = \frac{4^k \cdot c - b}{4^k - 1}$$

Very accurate & efficient if integral reasonably well behaved.

Classical Error Analysis

In one interval:



$$\int_a^b f_t\,dt = \frac{h}{2}\left(f_a + f_b\right) + E$$

← error

Use Taylor's Series with remainder:

$$f_t = f_a + (t-a) f_a' + \frac{(t-a)^2}{2!} f_\theta'' \qquad \text{for some } a \le \theta \le b$$

$$LHS = \int_a^b [\quad] dt = (b-a) f_a + \frac{(b-a)^2}{2} f_a' + \frac{(b-a)^3}{3!} f_\theta''$$

$$= RHS = \frac{h}{2}\left[f_a + f_a + (b-a) f_a' + \frac{(b-a)^2}{2!} f_\theta'' \right] + E$$

$$\cancel{h f_a} + \cancel{\frac{h^2}{2} f_a'} + \frac{h^3}{6} f_\theta'' = \cancel{h f_a} + \cancel{\frac{h^2}{2} f_a'} + \frac{h^3}{4} f_\theta'' + E$$

$$\Longrightarrow \qquad E = h^3\left(\frac{1}{6} - \frac{1}{4}\right) f_\theta''$$

$$\boxed{E = -\frac{h^3}{12} f_\theta''} \qquad \theta \in [a,b]$$

(small subinterval)

Extended Rule

$$E_{TOTAL} = -\frac{h^2}{12}\left[\sum_{\substack{\text{intervals}\\ i}} h f_{\theta_i}''\right] = -\frac{h^2}{12}(b-a) f_\theta'' \qquad \theta \in [a,b]$$

(uses mean value theorem, see [Atkinson 85]) this predicts that as we continue to halve h,

$$E_{new} \approx \frac{1}{4} E_{old}$$

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* the derivation assumes f is sufficiently smooth, that higher derivatives used are continuous.

Estimate [Atkinson85]:

$$E_{TOTAL} = \frac{-h^2}{12}\Bigg[\underbrace{\sum_{\substack{\text{intervals}\\ i}} h f''_{\theta_i}}_{\xrightarrow[h \to 0]{} \int_a^b f''(x)\,dx \,=\, f'(b) - f'(a)}\Bigg]$$

$$\boxed{E_{TOTAL} \approx -\frac{h^2}{12}\left[f'(b) - f'(a)\right]}$$

two implications:

1) can be much better if $f'(b) = f'(a)$

2) Suggests correcting result by this estimate.

Corresponding Result for Simpson's Rule

$$E_{TOTAL} = -\frac{h^4 (b-a) f^{(iv)}(\theta)}{90} \qquad \theta \in [a,b]$$

$$\approx -\frac{h^4}{90}\left[f'''(b) - f'''(a)\right]$$

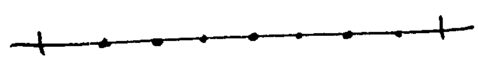
For smooth enough fctns, then, error is decreased by about $1/2^4 = 1/16$ each halving of h.

More Advanced Techniques:

Gauss quadrature Uses non-equally spaced points

Much more complicated!
Much more accurate in appropriate cases.

"open formulas"



uses only internal points.

Common Problems that require some thought:

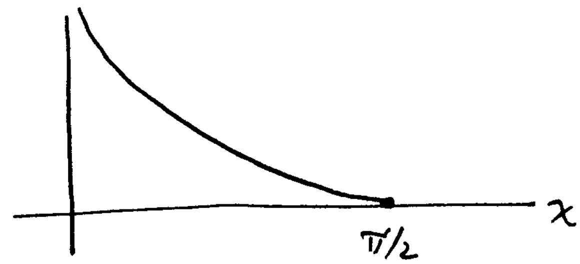
$$\int_A^{\infty} p(x)\,dx \qquad \text{infinite limit}$$

→ I want you to deal with this in Assignment 2. think!

"Sick" integrals (Strongly recommend [Acton 96])

e.g.

$$I = \int_0^{\pi/2} \frac{\cos x}{\sqrt{x}}\,dx$$

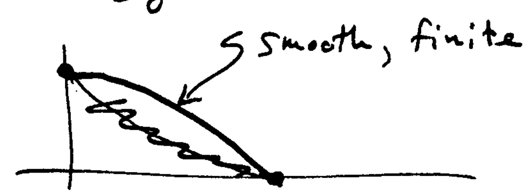


But nothing really bad is happening near $x = 0$, because

$$\int_0^{\pi/2} \frac{1}{\sqrt{x}}\,dx \quad \text{is } \underline{\text{finite}}.$$

the infinity can be removed; let $x = u^2$, $dx = 2u\,du$

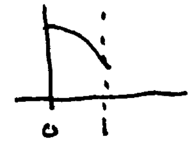
$$I = \int_0^{\sqrt{\pi/2}} \frac{\cos(u^2)}{\cancel{u}} \cdot 2\cancel{u}\,du = 2\int_0^{\sqrt{\pi/2}} \cos(u^2)\,du$$



$\sqrt{\ }$ & logs can often be fixed this way if they produce an infinity.

Examples of error behavior (Atkinson 85)

$$I^{(1)} = \int_0^1 e^{-x^2}\,dx \doteq 0.746\,824\,132\,812\,34$$



n = # pts.	Error – Trapezoidal	ratio	Error – Simpson's	ratio
2	1.55 E−2		−2.56 E−4	
4	3.84 E−3	4.02	−3.12 E−5	11.4
8	9.59 E−4	4.01	−1.99 E−6	15.7
16	2.40 E−4	4.00	−1.25 E−7	15.9
32	5.99 E−5	4.00	−7.79 E−9	16.0

$$I^{(3)} = \int_0^{2\pi} \frac{dx}{2+\cos(x)} = \frac{2\pi}{\sqrt{3}} \doteq 3.6275\,987\,284\,684$$

n = # pts.	Error – Trapezoidal	ratio	Error – Simpson's	ratio
2	−5.61 E−1		−1.26	
4	−3.76 E−2	14.9	1.37 E−1	−9.2
8	−1.93 E−4	195	1.23 E−2	11.2
16	−5.19 E−9	37600	6.43 E−5	191
32	* (machine limit)		1.71 E−9	37600
64	*		*	

why so good!

LESS ACCURATE!

$$I = \int_0^1 \sqrt{x}\,dx = 2/3$$

n = # pts.	Error – Simpson's	ratio
2	2.860 E−2	
4	1.012 E−2	2.82
8	3.587 E−3	2.83
16	1.268 E−3	2.83
32	4.485 E−4	2.83

← bad accuracy…

why so bad?