

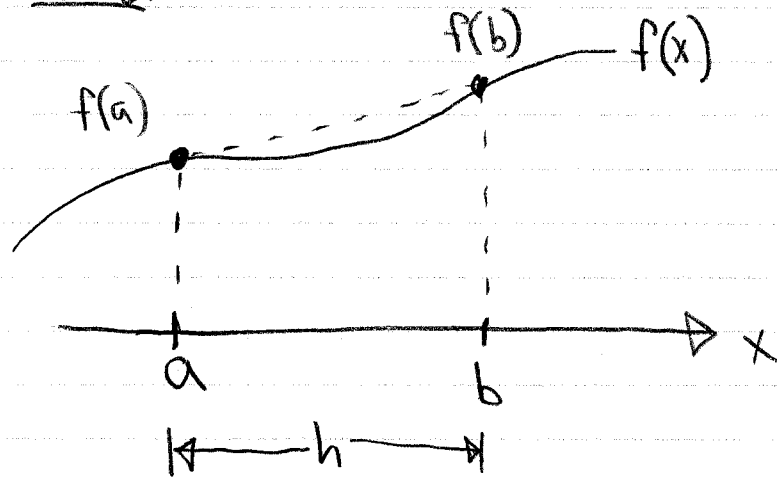
# NUMERICAL INTEGRATION (QUADRATURE — NR CH. 4)

WE ASSUME THAT WE HAVE A PROGRAM CAPABLE OF EVALUATING  $f(x)$  FOR AN ARBITRARY  $x$  (OR PREFERABLY, FOR AN ARRAY OF  $x$  VALUES IF WE ARE IN OCTAVE/MATLAB).

WE WISH TO ESTIMATE THE VALUE OF

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

FOR THE SIMPLEST CASE, WITH  $b$  CLOSE TO  $a$ , WE MIGHT FORM A CRUDE ESTIMATE USING THE TRAPEZOID RULE:



$$\int_a^b f(x) dx \approx \left( \frac{f(a) + f(b)}{2} \right) h.$$

THE EXTENDED TRAPEZOID RULE INVOLVES DIVIDING THE INTERVAL INTO  $N$  EQUAL SUB-INTERVALS:

• LET  $h = (b-a)/N$

$x_1 = a$

$x_2 = a+h$

⋮

$x_n = a + (n-1)h$

⋮

$x_N = a + (N-1)h$

$x_{N+1} = a + Nh = b.$

THERE WILL BE  $N+1$  EVALUATIONS OF  $f(x)$ :

$f_n = f(x_n).$

NOW USE THE TRAPEZOID RULE ON EACH SUB-INTERVAL:

$$\int_a^b f(x) dx = \sum_{n=1}^N \int_{x_n}^{x_{n+1}} f(x) dx$$

$$\approx h \sum_{n=1}^N \left( \frac{f_n + f_{n+1}}{2} \right) \quad (\text{TRAPEZOID RULE})$$

$$= h \left( \frac{f_1 + f_2}{2} + \frac{f_2 + f_3}{2} + \dots + \frac{f_{N-1} + f_N}{2} + \frac{f_N + f_{N+1}}{2} \right)$$

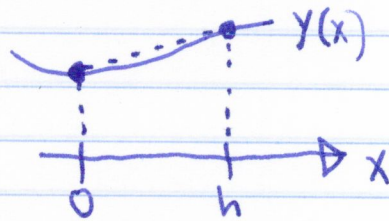
$$\int_{x_1}^{x_{N+1}} f(x) dx = h \left( \frac{f_1}{2} + \frac{f_{N+1}}{2} + \sum_{n=2}^N f_n \right)$$

EXTENDED TRAPEZOID RULE

### ERROR ANALYSIS

CONSIDER A SINGLE TRAPEZOID RULE STEP:

$$\int_0^h y dx$$



NOW LET  $y = a + bx + cx^2 + dx^3 + \dots$

THE TRAPEZOID RULE ESTIMATES:

$$\int_0^h y dx \approx \frac{h}{2} (y(0) + y(h)) = ah + \frac{b}{2}h^2 + \frac{c}{2}h^3 + \frac{d}{2}h^4 + \dots$$

THE EXACT ANSWER IS:

$$\int_0^h y dx = \left[ ax + \frac{1}{2}bx^2 + \frac{1}{3}cx^3 + \frac{1}{4}dx^4 + \dots \right]_0^h$$

$$= ah + \frac{1}{2}bh^2 + \frac{1}{3}ch^3 + \frac{1}{4}dh^4 + \dots$$

THE ERROR IS THE DIFFERENCE; TO LOWEST ORDER IN  $h$ ,

$$\text{ERR} \approx \frac{1}{6}ch^3 = \frac{1}{12}y''(0)h^3.$$

OVER AN INTERVAL WITH  $N$  STEPS ( $Nh = (b-a)$ ),

$$\text{EXTENDED ERR} = \frac{1}{12}y''h^3 \cdot N = \frac{y''}{12} \frac{(b-a)^3}{N^2}$$

$$\sim O\left(\frac{1}{N^2}\right).$$

THIS IS CALLED TRUNCATION ERROR. IN EFFECT, THE TRAPEZOID RULE TRUNCATES THE TAYLOR SERIES FOR  $y(x)$  OVER EACH SUB-INTERVAL.

WHAT ARE THE LIMITATIONS OF THE TRAPEZOID RULE?  
(HOW MIGHT IT FAIL?)

- ① TRUNCATION ERROR (SEE ABOVE)
- ② ROUND OFF ERROR (WE'LL TALK ABOUT THIS LATER)
- ③ IMPROPER INTEGRALS

EXAMPLE 1

CONSIDER  $\int_0^1 \frac{dx}{\sqrt{x}}$  — AN "IMPROPER" INTEGRAL.

ANALYTICALLY:

$$\int_0^1 x^{-1/2} dx = 2x^{1/2} \Big|_0^1 = 2.$$

TRAPEZOID RULE:  $f_n = \frac{1}{\sqrt{x_n}}$   
 $f_1 = \frac{1}{\sqrt{0}} \rightarrow \infty$

EXAMPLE 2

ANOTHER SORT OF IMPROPER INTEGRAL:

$$\int_1^\infty \frac{dx}{x^{3/2}} = \frac{2}{\sqrt{x}} \Big|_1^\infty = 2.$$

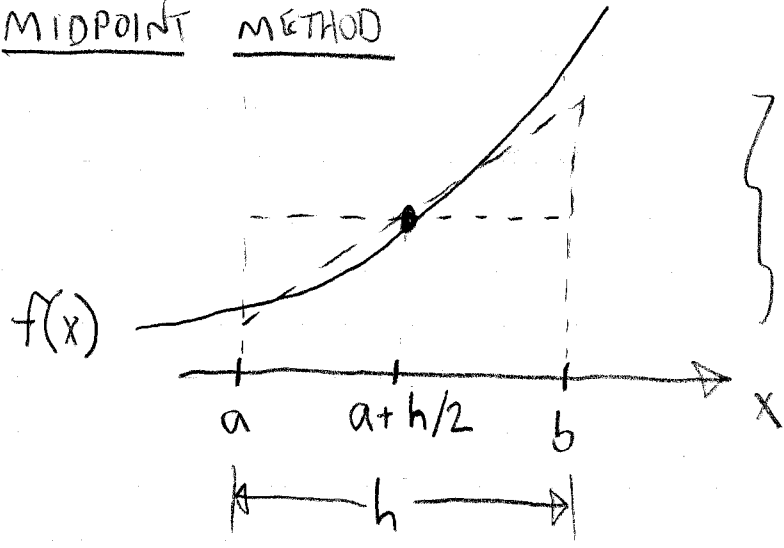
Q: HOW CAN WE DO THIS NUMERICALLY?

A: NEW VARIABLE: LET  $z = 1/x$ ,  $dx = -dz/z^2$

$$\int_1^\infty \frac{dx}{x^{3/2}} = - \int_1^0 \frac{z^{3/2}}{z^2} dz = \int_0^1 \frac{dz}{\sqrt{z}} \text{ — OH NO!}$$

- SOLVES THE PROBLEM OF  $\infty$  LIMITS
- CREATES A NEW IMPROPER INTEGRAL, WHICH THE TRAPEZOID RULE CANNOT SOLVE,
- FOR INTEGRANDS WITH SINGULARITIES AT THE ENDS, WE WANT AN OPEN QUADRATURE METHOD

# THE MIDPOINT METHOD



NOTE THAT THE DASHED RECTANGLE AND TRAPEZOID HAVE THE SAME AREA.

$$\int_a^b f(x) dx \approx h f(a + h/2), \quad h = (b - a)$$

EXTENDED MIDPOINT METHOD:  
 LET  $x_n = a + (n - \frac{1}{2})h$ ,  $h = (b - a) / N$   

$$\int_a^b f(x) dx \approx h \sum_{n=1}^N f(x_n)$$

- THE MIDPOINT METHOD IS OPEN IN THE SENSE THAT IT DOES NOT EVALUATE  $f(x)$  AT THE ENDS ( $x = a, b$ ).
- THEREFORE, THE MIDPOINT METHOD WILL NOT FAIL CATASTROPHICALLY IF THERE IS AN INTEGRABLE SINGULARITY AT  $a$  OR  $b$ .
- I HAVE 3 IMPLEMENTATIONS:

- midpoint 0.m — SLOW.
- midpoint 1.m — CAN RUN OUT OF MEMORY (LARGE N).
- midpoint 2.m — COMPROMISE BETWEEN SPEED AND MEMORY USE.

Q: HOW DOES TRUNCATION ERROR OF THE MM COMPARE TO TRAPEZOID?

EXAMPLES WITH INTEGRAND  $1/\sqrt{x}$  SHOW VERY SLOW CONVERGENCE. BUT THERE ARE A VARIETY OF WAYS TO TRANSFORM IMPROPER INTEGRALS TO FORMS THAT CAN BE INTEGRATED MORE EFFICIENTLY. EXAMPLE:

(6)

$$f(x) \equiv \int_0^x \frac{dx'}{\sqrt{\sin x'}}, \quad 0 \leq x \leq \pi$$

FOR SMALL  $x$ ,  $f(x) \approx g(x) \equiv \int_0^x \frac{dx'}{\sqrt{x'}} = 2\sqrt{x}$ .

LET US REWRITE  $f(x)$  THIS WAY:

$$\begin{aligned} f(x) &= f(x) - g(x) + g(x) \\ &= \int_0^x \left[ \frac{1}{\sqrt{\sin x'}} - \frac{1}{\sqrt{x'}} \right] dx' + 2\sqrt{x} \end{aligned}$$

WE STILL CAN'T EVALUATE THE INTEGRAND NUMERICALLY AT  $x'=0$ , BUT WITH AN OPEN SCHEME WE DON'T NEED TO. THE INTEGRAND IS NOW MUCH BETTER BEHAVED IN THE LIMIT  $x' \downarrow 0$ , THOUGH TAKING DIFFERENCES OF BIG NUMBERS DOES INCREASE ROUND OFF ERROR.

NOW, WHAT ABOUT  $x \uparrow \pi$ ?  $\sin x \rightarrow \pi - x$ , SO CONSIDER

$$h(x) \equiv \int_0^x \frac{dx'}{\sqrt{\pi - x'}} = -2\sqrt{\pi - x'} \Big|_0^x = 2(\sqrt{\pi} - \sqrt{\pi - x}).$$

LET  $f(x) = f(x) - h(x) + h(x)$ , AND

$$\begin{aligned} f(x) &= \int_0^x \left[ \frac{1}{\sqrt{\sin x'}} - \frac{1}{\sqrt{x'}} - \frac{1}{\sqrt{\pi - x'}} \right] dx' \\ &\quad + 2(\sqrt{x} + \sqrt{\pi} - \sqrt{\pi - x}). \end{aligned}$$

THE INTEGRAND IS NEARLY FLAT OVER  $0 \leq x' \leq \pi$ :

