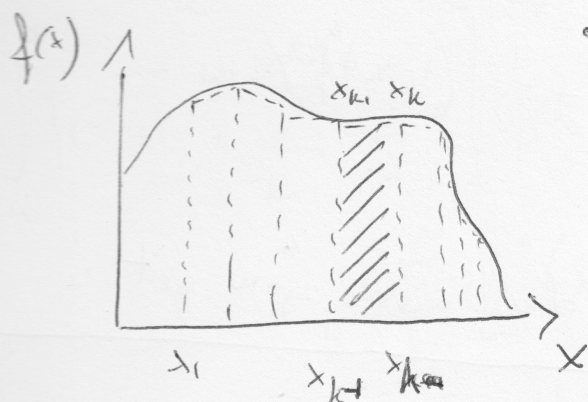


# NUMERICAL METHODS

## THEORY

### 1) Error estimation in trapezoidal rule for integrals



•) Consider slice  $[x_{k-1}, x_k]$  as in figure

Now Taylor expand  $f(x)$  around

$x_{k-1}$ :

$$f(x) = f(x_{k-1}) + (x - x_{k-1})f'(x_{k-1}) + \frac{1}{2}(x - x_{k-1})^2 f''(x_{k-1}) + \dots$$

•) Now integrate in the  $///$  area

$$\int_{x_{k-1}}^{x_k} f(x) dx = \int_{x_{k-1}}^{x_k} f(x_{k-1}) dx + \int_{x_{k-1}}^{x_k} (x - x_{k-1}) f'(x_{k-1}) dx + \frac{1}{2} \int_{x_{k-1}}^{x_k} (x - x_{k-1})^2 f''(x_{k-1}) dx + \dots$$

$+ \dots$

•) Now assume that the size of each step is  $h$ , that is  $|x_k - x_{k-1}| = h$   
 Make the substitution  $|x - x_{k-1}| = u \Rightarrow du = dx$ .

We get

$$\int_{x_{k-1}}^{x_k} f(x) dx = f(x_{k-1}) \int_0^h du + f'(x_{k-1}) \int_0^h u du + \frac{1}{2} f''(x_{k-1}) \int_0^h u^2 du + \dots$$

→) Trace pre:

$$\int_{x_k}^{x_{k+1}} f(x) dx = f(x_{k-1})h + \frac{1}{2}f'(x_{k-1})h^2 + \frac{1}{6}h^3 f''(x_{k-1}) + O(h^4) \quad (\star)$$

•) Now, expand around  $x_k$

$$f(x) \approx f(x_k) + (x - x_k) f'(x_k) + \frac{1}{2}(x - x_k)^2 f''(x_k) + \dots$$

Integrate as before

$$\int_{x_{k-1}}^{x_k} f(x) dx = \int_{x_{k-1}}^{x_k} f(x_k) dx + \int_{x_{k-1}}^{x_k} (x - x_k) f'(x_k) dx + \frac{1}{2} \int_{x_{k-1}}^{x_k} (x - x_k)^2 f''(x_k) dx + \dots$$

Replace again  $x - x_k = u$ ,  $dx = du$ . We now get

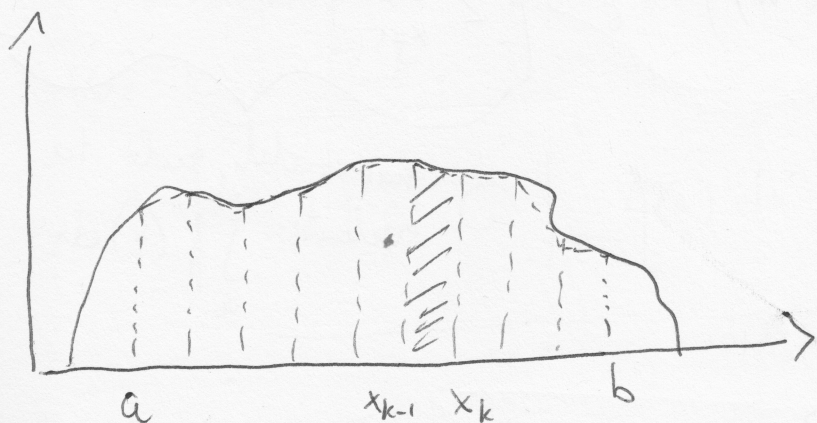
$$\begin{aligned} \int_{x_{k-1}}^{x_k} f(x) dx &= \int_{-h}^0 f(x_k) dx + \int_{-h}^0 u f'(x_k) du + \frac{1}{2} \int_{-h}^0 u^2 f''(x_k) du + \dots \\ &= f(x_k)h + \frac{1}{2}f'(x_k)h^2 + \frac{1}{6}f''(x_k)h^3 + O(h^4) \quad (\star) \end{aligned}$$

•) ~~Now~~ Now sum  $(\star) + (\star)$  to get

$$\begin{aligned} 2 \int_{x_{k-1}}^{x_k} f(x) dx &= [f(x_k) + f(x_{k-1})]h + \frac{1}{2}[f'(x_{k-1}) - f'(x_k)]h^2 \\ &\quad + \frac{1}{6}[f''(x_{k-1}) + f''(x_k)]h^3 + O(h^4) \end{aligned}$$



•) We can then write  $\int_a^b f(x) dx = \sum_{k=1}^N \int_{x_{k-1}}^{x_k} f(x) dx$



Summing the R.H.S of the last equation we arrive at:

$$\int_a^b f(x) dx = \sum_{k=1}^N \frac{1}{2} h [f(x_k) + f(x_{k-1})] + \frac{1}{4} h^2 \sum_{k=1}^N [f'(x_{k-1}) - f'(x_k)] + \frac{1}{12} h^3 \sum_{k=1}^N [f''(x_{k-1}) + f''(x_k)] + O(h^4)$$

Now we see that  $\sum_{k=1}^N [f'(x_{k-1}) - f'(x_k)] = f'(a) - f'(a+h) + f'(a+h) - f'(a+2h) + f'(a+2h) - f'(a+3h) + \dots - f'(b) = f'(a) - f'(b)$

•) Therefore:

$$\int_a^b f(x) dx = \frac{1}{2} h \sum_{k=1}^N [f(x_k) + f(x_{k-1})] + \frac{1}{4} h^2 [f'(a) - f'(b)] + \frac{1}{12} h^3 \sum_{k=1}^N [f''(x_{k-1}) + f''(x_k)] + O(h^4)$$

Now note that  $\frac{1}{2} h \sum_{k=1}^N [f(x_k) + f(x_{k-1})]$  is exactly the trapezoidal rule

Therefore  $\text{ERROR} = \frac{1}{4} h^2 [f'(a) - f'(b)] + \frac{1}{12} h^3 \sum_{k=1}^N [f''(x_{k-1}) + f''(x_k)] + O(h^4)$

.) Now look at the error formula and focus on the term

$$\frac{1}{12} h^3 \sum_{k=1}^N \left( f''(x_{k-1}) + f''(x_k) \right) = \frac{h^2}{6} \cdot \underbrace{\left[ \frac{h}{2} \sum_{k=1}^N \left( f''(x_{k-1}) + f''(x_k) \right) \right]}_{\text{trapezoidal rule to evaluate } \int_a^b f''(x) dx}$$

We can then write

$$\begin{aligned} \frac{h^2}{6} [ \quad ] &= \frac{h^2}{6} \left[ \int_a^b f''(x) dx + O(h^2) \right] = \\ &= \frac{h^2}{6} \left( f'(b) - f'(a) \right) + O(h^4) \end{aligned}$$

.) We replace the latest expression in the error formula, at the end of previous page, to get:

$$\text{ERROR} \equiv \mathcal{E}_{\text{trapezoid}} = \frac{1}{12} h^2 \left[ f'(a) - f'(b) \right] + \frac{1}{6} h^2 \left[ f'(b) - f'(a) \right] + O(h^4)$$

$$\Rightarrow \boxed{\mathcal{E}_{\text{trap.}} = \frac{1}{12} h^2 \left[ f'(a) - f'(b) \right] + O(h^4)}$$

This is the error introduced by approximating the  $\int$  with sums over trapezoids. It scales like  $h^2$ , where  $h$  is the size of the bin, that is  $h = \frac{b-a}{N}$ , with  $N = \text{number of points}$



- .) If we increase  $N$  and decrease  $h$ , we get higher accuracy in the result, This is until we hit machine precision that is  $\epsilon_{\text{trapezoidal}} = \epsilon_{\text{round}}$ , where  $\epsilon_{\text{round}}$  is the rounding error.

We know that:

$$\left[ \epsilon_{\text{round}} \approx C \int_a^b f(x) dx ; C \approx 10^{-16} \right]$$

- .) Imposing  $\epsilon_{\text{trapezoidal}} = \epsilon_{\text{round}}$  we get

$$\frac{1}{12} h^2 [f'(a) - f'(b)] = C \int_a^b f(x) dx$$

Solve for  $h$ :

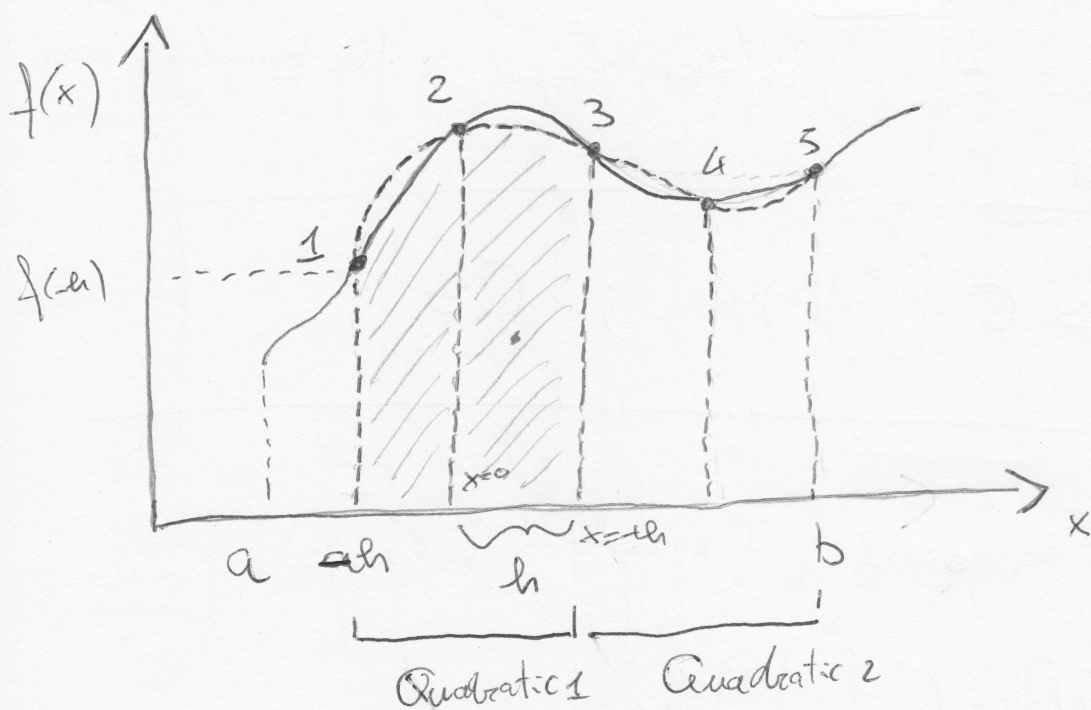
$$h = \left[ \frac{12 \int_a^b f(x) dx}{f'(a) - f'(b)} \right]^{\frac{1}{2}} C^{\frac{1}{2}}$$

Since  $h = \frac{b-a}{N}$  we can solve for  $N$ :

$$\left[ N = \left[ \frac{f'(a) - f'(b)}{12 \int_a^b f(x) dx} \right]^{\frac{1}{2}} (b-a) C^{-\frac{1}{2}} \right]$$

Roughly, we hit machine precision with  $N \approx C^{\frac{1}{2}} \approx 10^8$

# SIMPSON'S RULE



.) Fit a quadratic through pts. 1, 2, 3, then 3, 4, 5, etc...

i) Consider points 1, 2, 3 and fit the curve  $Ax^2 + Bx + C$   
 We assign (no loss of generality) coordinate  $x=0$  in point 2. Therefore  $x=-h$  in 1 and  $x=h$  in 3

$$\begin{cases} \ln 1: f(-h) = Ah^2 - Bh + C \\ \ln 2: f(0) = C \\ \ln 3: f(h) = Ah^2 + Bh + C \end{cases}$$

Therefore: 2)  $f(h) = Ah^2 + Bh + f(0)$ ;  $Ah^2 = f(h) - f(0) - Bh$

2)  $\Rightarrow$   $f(-h) = f(h) - f(0) - 2Bh$

$$B = \frac{f(h) - f(-h)}{2h}$$

3)  $\Rightarrow f(h) = Ah^2 + \frac{f(h) - f(-h)}{2} + f(0)$



$$A = \frac{1}{h^2} \left[ f(h) - \frac{f(h) - f(-h)}{2} - f(0) \right] = \frac{1}{h^2} \left[ \frac{f(h) - f(-h)}{2} - f(0) \right]$$

ii) Now that we have  $A, B, C$ , approximate the integral  $\int_{-h}^h$  (shaded area) with the area under the quadratic

$$\int_{-h}^h f(x) dx \approx \int_{-h}^h (Ax^2 + Bx + C) dx = \left. \frac{1}{3} Ax^3 + \frac{1}{2} Bx^2 + Cx \right|_{-h}^h$$

$$= \frac{2}{3} Ah^3 + 2Ch = \frac{2}{3} \frac{1}{h^2} \left[ \frac{f(h) - f(-h)}{2} - f(0) \right] h^3 + 2hf(0)$$

$$= \frac{2h}{3} \frac{f(h)}{2} + \frac{2h}{3} \frac{f(-h)}{2} - \frac{2f(0)}{3} h + 2hf(0) =$$

$$= \frac{h}{3} f(h) + \frac{h}{3} f(-h) + \frac{4h}{3} f(0) \Rightarrow$$

$$\int_{-h}^h f(x) dx \approx \frac{1}{3} h [f(h) + f(-h) + 4f(0)]$$

iii) Therefore, for any interval of length  $2h$ , fitting the quadratic between the points  $x_{k-1}, x_k, x_{k+1}$  we get

$$\int_{x_{k-1}}^{x_{k+1}} f(x) dx \approx \frac{1}{3} h [f(x_{k-1}) + 4f(x_k) + f(x_{k+1})]$$

Now sum to get  $\int_a^b f(x) dx \approx \sum_{k=1}^N \frac{1}{3} h [f(x_{k-1}) + 4f(x_k) + f(x_{k+1})]$

$$\begin{array}{c}
 x_n = a + nh \\
 \hline
 x_0 = a \quad x_1 = a+h \quad x_2 = a+2h \quad \dots \quad x_n = a+nh
 \end{array}$$

iv) If we indicate  $x_n = a + nh$  we see that

$\left\{ \begin{array}{l} n \text{ even} \Rightarrow \text{first and last point in each 3 point interval} \\ n \text{ odd} \Rightarrow \text{central point in each 3 point interval} \end{array} \right.$

So we get:

$$\int_a^b f(x) dx = \frac{1}{3} h \left[ \underbrace{f(a) + 4f(a+h) + f(a+2h)}_{\text{INTERVAL 1}} + 4f(a+3h) + \dots + f(b) \right] \Rightarrow$$

$$\int_a^b f(x) dx \approx \frac{4h}{3} \sum_{\substack{k=1 \\ k \text{ odd}}}^{N-1} f(a+kh) + \frac{2h}{3} \sum_{\substack{k=2 \\ k \text{ even}}}^{N-2} f(a+kh) + f(a) + f(b)$$

↑↑

SIMPSON'S RULE

iv) A similar (more cumbersome) procedure to the one showed for trapezoidal leads to the error

$$\left[ \varepsilon = \frac{h^4}{180} [f'''(a) - f'''(b)] \right]$$



This goes like  $h^4$ , much better ( $h \ll 1$ ) than  $\mathcal{E} \propto h^2$ , which we were getting for trapezoidal. By setting  $\mathcal{E} = C \int_a^b f(x) dx$ , with machine precision  $C \approx 10^{-16}$ , we see the Simpson's method hits machine precision with  $N \approx 10^4$  points in the sample (it was  $N \approx 10^8$  with trapezoidal), provided 3<sup>rd</sup> derivatives of  $f$  are not very large.

## ROMBERG INTEGRATION

i) Consider trapezoidal rule. Sample the  $[a, b]$  interval with  $N_i$  points, say that  $I_i$  is the result of the numerical integral and  $I$  is the exact one. We know that

$$I = I_i + \underbrace{a h_i^2}_{\text{numerical error}} = I_i + \mathcal{E}_i$$

Now recompute the integral with more points. Call it  $I_{i+1}$  (with  $N_{i+1}$  points). Again

$$I = I_{i+1} + a h_{i+1}^2 = I_{i+1} + \mathcal{E}_{i+1}$$

If we take  $N_{i+1} = 2N_i$  then  $h_{i+1} = \frac{1}{2} h_i$  and

$$\begin{aligned} 1) \int I &= I_i + a h_i^2 \\ 2) \int I &= I_{i+1} + \frac{1}{4} a h_i^2 \end{aligned} \Rightarrow \frac{1}{4} a h_i^2 = I - I_{i+1} \quad 1)$$

$$= I_i - a h_i^2 - I_{i+1}$$

$$\text{So } I_{i+1} - I_i = \frac{3}{4} a h_i^2 = 0$$

$$(I_{i+1} - I_i) = \frac{3}{4} a h_i^2 = 3a h_{i+1}^2$$

( $h_{i+1} = \frac{1}{2} h_i$ )

This goes like  $h^4$ , much better ( $h \ll 1$ ) than  $\epsilon \sim h^2$ , which we were getting for trapezoidal. By setting  $\epsilon = C \int_a^b |f(x)| dx$ , with machine precision  $C \approx 10^{-16}$ , we see the Simpson's method hits machine precision with  $N \approx 10^4$  points in the sample (it was  $N \approx 10^8$  with trapezoidal), provided 3<sup>rd</sup> derivatives of  $f$  are not very large.

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( $h_{i+1} = \frac{1}{2} h_i$ )



Therefore  $I_{i+1} - I_i = 3 \epsilon_2$ ,  $\left| \epsilon_2 = \frac{1}{3} (I_{i+1} - I_i) \right|$  (Trapezoidal)

I can iterate trapezoidal by doubling the number of points at each step, and get an estimate of the error.

I could do the same for Simpson's, getting (check it!)

$$\left| \epsilon_2 = \frac{1}{15} (I_2 - I_1) \right| \text{ (Simpson)}$$

ii) Now say you computed trapezoidal to get  $I_1$  with  $N_1$  points

$$I = I_1 + a h^2 = I_1 + \epsilon_1$$

Now we double the number of points to get

$$I = I_2 + \epsilon_2 ; \epsilon_2 \sim O(h^2)$$

But we can explicitly write  $\epsilon_2 = \frac{1}{3} (I_2 - I_1)$  and

$$I = I_2 + \frac{1}{3} (I_2 - I_1) + \underline{\underline{O(h^4)}}$$

We combined two trapezoidal and "skipped" to the  $O(h^4)$  term in the error expansion, making trapezoidal as accurate as Simpson's. The idea of Romberg method is to iterate this approach.

iii) At the  $i^{\text{th}}$  iteration, say we have  $I_i$ , We define

$$R_{i,1} \equiv I_i$$

At the iteration before we had  $I_{i-1}$  ( $N_{i-1} = \frac{N_i}{2}$ )

Therefore  $I_{i+1} - I_i = 3 \epsilon_2$ ,  $\left| \epsilon_2 = \frac{1}{3} (I_{i+1} - I_i) \right|$  (Trapezoidal)

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and we build:  $R_{i,2} = I_i + \frac{1}{3}(I_i - I_{i-1})$

As we saw:  $I = \underset{\substack{\downarrow \\ \text{true value}}}{R_{i,2}} + O(h_i^4)$ . Let's write explicitly:

$$I = R_{i,2} + a_2 h_i^4 + O(h_i^6)$$

•) At the order  $(i-1)$  of the iteration we had analogously computed  $R_{i-1,1} = I_{i-1}$  and  $R_{i-1,2} = I_{i-1} + \frac{1}{3}(I_{i-1} - I_{i-2})$  and we know that  $R_{i-1,2} + O(h_{i-1}^4) = I$

•) Let's then play the same trick with  $R_{i,2}$  and  $R_{i-1,2}$ !

$$\left\{ \begin{array}{l} I = R_{i,2} + a_2 h_i^4 + O(h_i^6) \\ I = R_{i-1,2} + a_2 h_{i-1}^4 + O(h_{i-1}^6) \end{array} \right.$$

$$I = R_{i-1,2} + a_2 h_{i-1}^4 + O(h_{i-1}^6) \stackrel{\substack{\downarrow \\ |h_{i-1} = 2h_i|}}{=} R_{i-1,2} + 16a_2 h_i^4 + O(h_i^6)$$

$\Downarrow$

$$R_{i,2} + a_2 h_i^4 + O(h_i^6) = R_{i-1,2} + 16a_2 h_i^4 + O(h_i^6) = 0$$

$$\Rightarrow \boxed{a_2 h_i^4 = \frac{1}{15}(R_{i,2} - R_{i-1,2}) + O(h_i^6)}$$

Now plug this into  $I = R_{i,2} + a_2 h_i^4 + O(h_i^6)$  to get

$$\boxed{R_{i,3} = R_{i,2} + \frac{1}{15}(R_{i,2} - R_{i-1,2}) + \cancel{O(h_i^6)}}$$

$R_{i,3}$  is now an estimate of  $I$  with error scaling like  $O(h_i^6)$ !  $\Rightarrow I = R_{i,3} + O(h_i^6) = R_{i,3} + a_3 h_i^6$

and we build:  $R_{i,2} = I_i + \frac{1}{3}(I_i - I_{i-1})$

As we saw:  $I = \underset{\substack{\downarrow \\ \text{true value}}}{R_{i,2}} + O(h_i^4)$ . Let's write explicitly:

$$I = R_{i,2} + a_2 h_i^4 + O(h_i^6)$$

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$$\begin{cases} I = R_{i,2} + a_2 h_i^4 + O(h_i^6) \\ I = R_{i-1,2} + a_2 h_{i-1}^4 + O(h_{i-1}^6) \end{cases}$$

$\Downarrow$

$\underbrace{\hspace{10em}}_{|h_{i-1} = 2h_i|}$

$$R_{i,2} + a_2 h_i^4 + O(h_i^6) = R_{i-1,2} + 16a_2 h_i^4 + O(h_i^6) = 0$$

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•) You can proceed recursively:

At each step you compute explicitly this column using  
 $\downarrow$  trapezoidal rule on doubling  $N$  w.r.t. previous step

$$I_1 \equiv R_{1,1} \quad (\varepsilon \sim O(h^2))$$

$$I_2 \equiv R_{2,1} \rightarrow R_{2,2} \quad (\varepsilon \sim O(h^4))$$

$$I_3 \equiv R_{3,1} \rightarrow R_{3,2} \rightarrow R_{3,3} \quad (\varepsilon \sim O(h^6))$$

$$I_4 \equiv R_{4,1} \rightarrow R_{4,2} \rightarrow R_{4,3} \rightarrow R_{4,4} \quad (\varepsilon \sim O(h^8))$$

$\vdots$  (The  $\rightarrow$  tells which estimates combine to get the next one in the current row)

•) Explicitly working out the recursion formula gives the expression:

$$R_{i,m+1} = R_{i,m} + \frac{1}{4^m - 1} (R_{i,m} - R_{i-1,m})$$

INTEGRALS OVER INFINITE RANGE

$$i) \int_0^\infty f(x) dx ; z = \frac{x}{1+x}, dx = \frac{dz}{(1-z)^2} \Rightarrow \int_0^1 \frac{1}{1-z} f\left(\frac{z}{1-z}\right) dz$$

$$ii) \int_a^\infty f(x) dx ; z = \frac{x-a}{1+xa}, dx = \frac{dz}{(1-z)^2} \Rightarrow \int_0^1 \frac{dz}{(1-z)^2} f\left(\frac{z}{1-z} + a\right)$$

$$iii) \int_{-\infty}^{+\infty} f(x) dx ; x = \tan(z), dx = \frac{dz}{\cos^2 z} \Rightarrow \int_{-\infty}^{+\infty} \frac{f(\tan z)}{\cos^2 z} dz$$

•) You can proceed recursively:

At each step you compute explicitly this sum using  
 $\downarrow$  trapezoidal rule on doubling  $N$  w.r.t. previous step

$$I_1 \equiv R_{1,1} \quad (\varepsilon \sim O(2^1))$$

$$I_2 \equiv R_{2,1} \rightarrow R_{2,2} \quad (\varepsilon \sim O(2^4))$$

$$I_3 \equiv R_{3,1} \rightarrow R_{3,2} \rightarrow R_{3,3} \quad (\varepsilon \sim O(2^9))$$

$$I_4 \equiv R_{4,1} \rightarrow R_{4,2} \rightarrow R_{4,3} \rightarrow R_{4,4} \quad (\varepsilon \sim O(2^{16}))$$

⋮  
 (The  $\rightarrow$  tells which estimates combine to get the next one in the ~~current~~ row)

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