Numerical Integration

Our objective is to design an algorithm which produces an approximation of the definite integral

$$I = \int_a^b f(x)\,dx.$$

The reasons why an approximation would be sought instead of an analytic computation, include:

→ The anti-derivative of f may not be expressible using fundamental functions, or

→ An anti-derivative may be too expensive to evaluate.

The general methodology for such an approximation is:

→ Introduce points $[x_k]_{k=0}^{N}$ such that

$$a = x_0 < x_1 < x_2 < \cdots < x_{N-1} < x_N = b$$

→ In every interval $[x_k, x_{k+1}]$, approximate $f(x)$ with a "simpler" function $p^{(k)}(x)$ which is trivial to integrate.

Approximate $I_k = \int_{x_k}^{x_{k+1}} f(x)\,dx \approx \int_{x_k}^{x_{k+1}} p^{(k)}(x)\,dx$

After I_k has been approximated, an approximation for the entire $I = \int_a^b f(x)dx = \sum_k I_k \approx \sum_k \int_{x_k}^{x_{k+1}} p^{(k)}(x)\,dx$ is assembled.

Next, we will see certain popular choices for $p^{(k)}(x)$

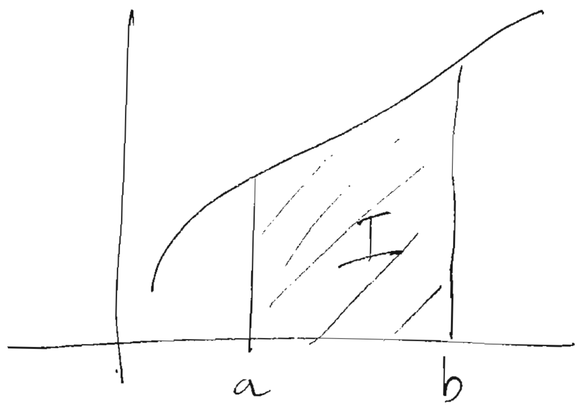
I. The rectangle rule

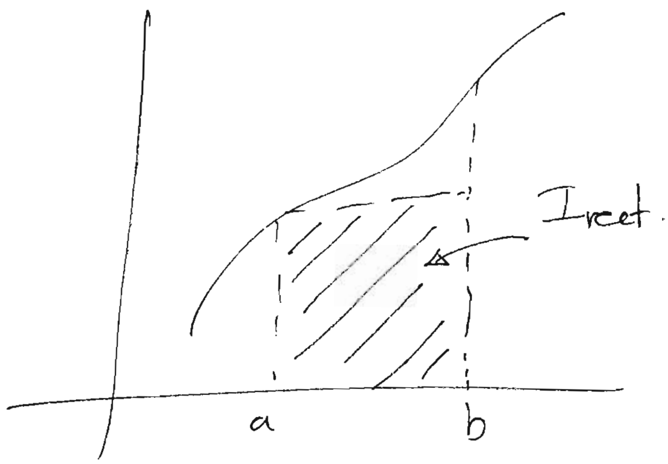
[First, we consider the entire interval $[a,b]$, without any partitioning, for simplicity of exposition].

The rectangle rule approximates $f(x) \approx f(a)$ (in $[a,b]$)

Thus $I = \int_a^b f(x)dx \approx \underbrace{\int_a^b f(a)\,dx}_{:= I_{rect}} = (b-a) f(a)$

Graphically:





In order to design a "composite" rectangle rule, we use the partition $a = x_0 < x_1 < \cdots < x_{N-1} < x_N = b$, and use the previous rule to approximate

$$I_k = \int_{x_k}^{x_{k+1}} f(x)\,dx \approx \underbrace{(x_{k+1} - x_k)\, f(x_k)}_{:= I_{k,rect}} = h_k\, f(x_k)$$

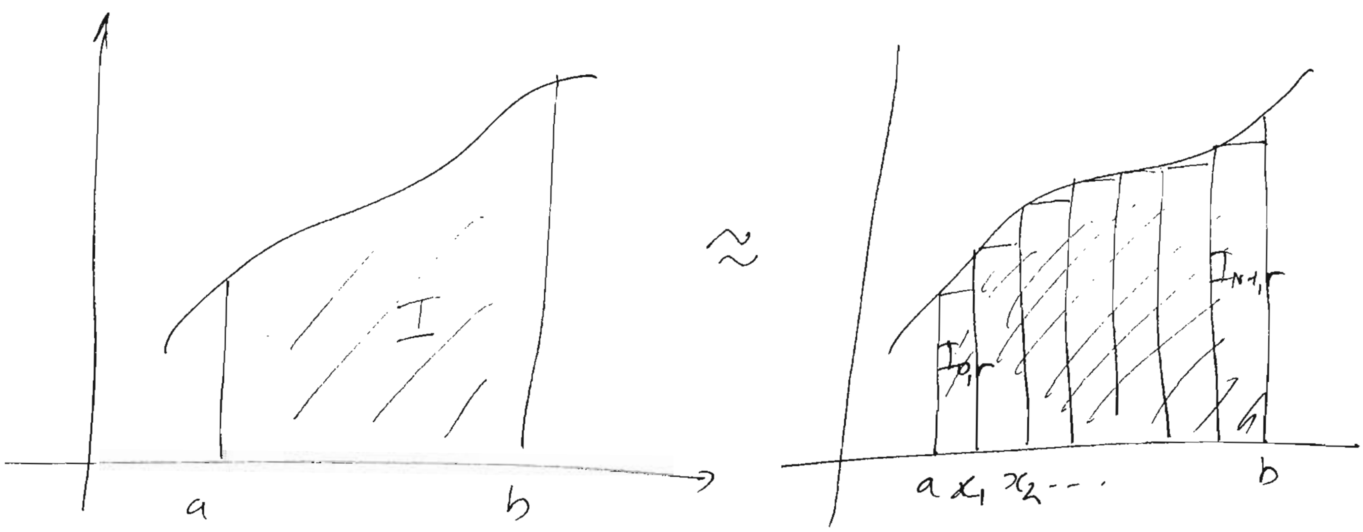
(where we defined $h_k := x_{k+1} - x_k$).

In the case where $h_0 = h_1 = h_2 = \cdots = h_{N-1} = h$ = const, we have

$$I = \int_a^b f(x)\,dx \approx \sum_{k=0}^{N-1} I_{k,rect} =$$

$$= \sum_{k=0}^{N-1} h \cdot f(x_k) = \underbrace{\frac{b-a}{N}}_{=h} \sum_{k=0}^{N-1} f(x_k)$$

Graphically:



As in the case of interpolation, we want 4/12/11 L
to be conscious about the <u>error</u> involved in this approximation. This, in fact, comes in 2 flavors:

→ The local error, is defined in each subinterval as:

$$e_k = \left| I_{k,\text{rule}} - I_{k,\text{analytic}} \right|.$$

For the rectangle rule, we have:

$$e_k = \left| \int_{x_k}^{x_{k+1}} f(x_k)\,dx - \int_{x_k}^{x_{k+1}} f(x)\,dx \right|$$

$$= \left| \int_{x_k}^{x_{k+1}} \left[f(x_k) - f(x) \right] dx \right| \qquad (1)$$

We shall seek to obtain an upper bound for the integral in eqn (1). Let us remember Taylor's formula, applied to $f(x)$ in the vicinity of x_k:

$$f(x) = f(x_k) + f'(c_k)(x - x_k), \quad \text{where } c_k \in (x_k, x_{k+1})$$

Thus

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$$e_K = \left| -\int_{x_K}^{x_{K+1}} f'(c_K)(x-x_K)\,dx \right|$$

$$\le \int_{x_K}^{x_{K+1}} |f'(c_K)|\,|x-x_K|\,dx$$

$$\le \int_{x_K}^{x_{K+1}} \|f'\|_\infty \underbrace{|x-x_K|}_{\geq 0}\,dx = \|f'\|_\infty \int_{x_K}^{x_{K+1}} (x-x_K)\,dx$$

$$= \|f'\|_\infty \left[\frac{(x-x_K)^2}{2}\right]_{x_K}^{x_{K+1}} = \frac{1}{2}\|f'\|_\infty \frac{(x_{K+1}-x_K)^2}{2}$$

$$\Rightarrow \boxed{e_K \le \frac{1}{2}\|f'\|_\infty \cdot h_K^2}$$

→ The global error is defined as:

$$e = |I_{rule} - I_{analytic}| = \left| \sum_{K=0}^{N-1} [I_{K,rule} - I_{K,analytic}] \right|$$

$$\le \sum_{K=0}^{N-1} |I_{K,rule} - I_{K,analytic}| = \sum_{K=0}^{N-1} e_K$$

For example, if $h = \text{const}$, for the rectangle rule we have:

$$e \le \sum_{K=0}^{N-1} e_K = N \cdot \frac{1}{2}\|f'\|_\infty \cdot h^2 \underset{Nh=b-a}{\Longrightarrow} \boxed{e_{global} \le \frac{b-a}{2}\|f'\|_\infty h}$$

What we observe is that, for the rectangle rule:

Local error $= O(h^2)$

Global error $= O(h)$

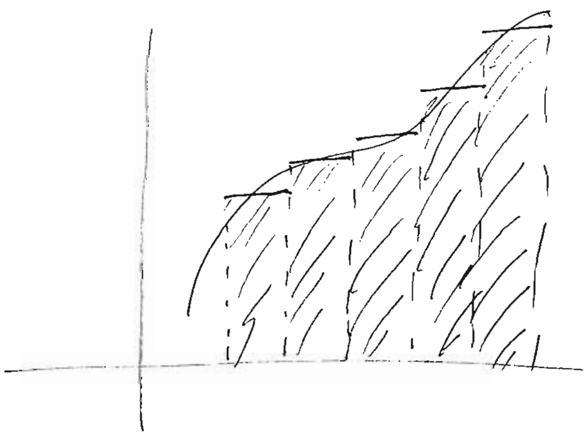
In general, we always get that if the local error is $O(h^{d+1})$ the global will be $O(h^d)$; additionally, in this case the numerical integration rule is called d-order accurate (e.g. rectangle rule is 1st order accurate)

II. Midpoint rule: $f(x) \approx f\left(\frac{x_k + x_{k+1}}{2}\right)$

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

Composite rule [h = constant]

$$I = \int_a^b f(x)\,dx \approx \sum_{k=0}^{N-1} \underbrace{(x_{k+1} - x_k)}_{=h=\frac{b-a}{N}} f\left(\frac{x_k + x_{k+1}}{2}\right) = \frac{b-a}{N} \sum_{k=0}^{N-1} f\left(\frac{x_k + x_{k+1}}{2}\right)$$



Local error analysis:

We use the (2nd order) Taylor's formula around the point $x_m = \frac{x_k + x_{k+1}}{2}$

$$f(x) = f(x_m) + f'(x_m)(x - x_m) + \frac{f''(c_k)}{2}(x - x_m)$$

$$c_k \in [x_k, x_{k+1}].$$

$$e_k = \left| \int_{x_k}^{x_{k+1}} [f(x_m) - f(x)]\, dx \right. =$$

$$= \left| f'(x_m) \int_{x_k}^{x_{k+1}} (x - x_m)\, dx + \int_{x_k}^{x_{k+1}} \frac{f''(c_k)}{2} (x - x_m)^2\, dx \right|$$

Note that $\displaystyle\int_{x_k}^{x_{k+1}} (x - x_m)\, dx = \left. \frac{(x - x_m)^2}{2} \right|_{x_k}^{x_{k+1}} = \frac{h_k^2}{8} - \frac{h_k^2}{8} = 0$

Thus:

$$e_k = \left| \frac{1}{2} \int_{x_k}^{x_{k+1}} f''(c_k)(x - x_m)^2\, dx \right| \leq \frac{1}{2} \int_{x_k}^{x_{k+1}} |f''(c_k)|\, |x - x_m|^2\, dx$$

$$\leq \frac{1}{2} \|f''\|_\infty \int_{x_k}^{x_{k+1}} (x - x_m)^2\, dx = \frac{1}{2} \|f''\|_\infty \left[\frac{(x - x_m)^3}{3} \right]_{x_k}^{x_{k+1}} =$$

$$= \frac{1}{2} \| f'' \|_\infty \left(\frac{h_k^3}{24} + \frac{h_k^3}{24} \right) \Rightarrow \boxed{e_k \leq \frac{1}{24} \| f'' \|_\infty h_k^3}$$

Global error :

$$e_{global} \leq \sum_{k=0}^{N-1} e_k \Rightarrow \boxed{e_k \leq \frac{b-a}{24} \| f'' \|_\infty \cdot h^2}$$

Thus, the midpoint rule is 2nd order accurate