



NTNU

Norwegian University of Science and Technology

TMA4130 Matematikk 4N

Week 35:

Interpolation and numerical integration

Douglas R. Q. Pacheco

Department of Mathematical Sciences, NTNU.

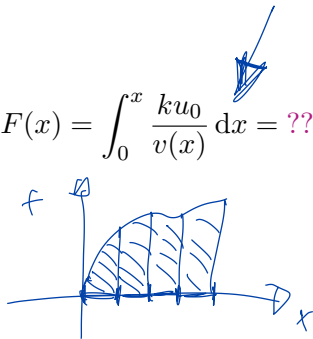
Autumn semester, 2022

Composite integration rules

Remember our motivation

Reactor, $a = 2$: $u(x) = \frac{u_0}{1 + F(x)}$, with $F(x) = \int_0^x \frac{ku_0}{v(x)} dx = ???$

$F(x_i) =$



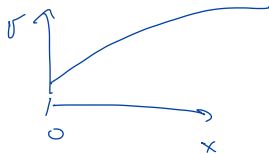
Composite rules are when I certain rule (defined for the interval $[a, b]$) is applied to smaller intervals $[x_i, x_{i+1}]$

Example

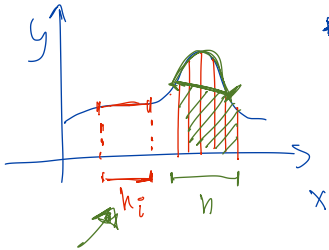
$$u(x) = \frac{u_0}{1 + F(x)}, \quad \text{with} \quad F(x) = \int_0^x \frac{ku_0}{v(x)} dx$$

Problem data: $L = 5, u_0 = 1, k = 1, v(x) = \ln(x + 2)$

$$F(x_i) = \int_0^{x_i} \frac{1}{\ln(x + 2)} dx$$

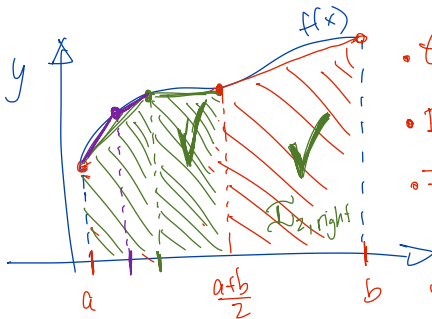


Adaptive integration



* We want to construct an automatic subdivision algorithm for the interval $[a, b]$, based on the integrand. But how to do that?

→ adaptivity



- Compute \mathcal{R}_1
 - Estimate the integration error (?)
 - If the error is too large, we can divide $[a, b]$ into two!
- Then I compute \mathcal{R}_2

Adaptive integration

Given f , a , b and a user-defined tolerance Tol.

1. Calculate $I(a, b)$ and estimate the error $\mathcal{E}(a, b)$,
2. **if** $|\mathcal{E}(a, b)| \leq \text{Tol}$
 - ▶ Accept the result,
 - ▶ return $I(a, b) + \mathcal{E}(a, b)$ as an approximation to $\int_a^b f(x) dx$.

else

- ▶ set $c = (a + b)/2$, and repeat the process on each of the subintervals $[a, c]$ and $[c, b]$, with tolerance Tol/2.
3. Sum up the accepted results from each subinterval.

Error estimation

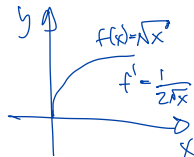
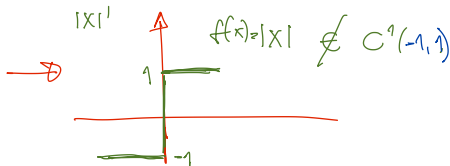
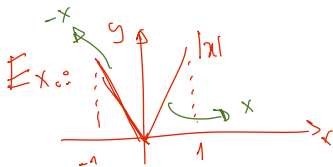
Trapezoidal rule: $I_T - \int_a^b f(x) dx = \frac{(b-a)^3}{12} f''(\xi)$ if $f \in C^2(a, b)$, $\xi \in [a, b]$

Error estimation

Trapezoidal rule: $I_T - \int_a^b f(x) dx = \frac{(b-a)^3}{12} f''(\xi)$ if $f \in C^2(a, b)$, $\xi \in [a, b]$

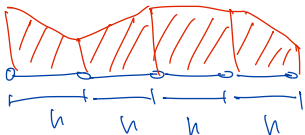
Simpson's rule: $I_S - \int_a^b f(x) dx = \frac{(b-a)^5}{2880} f^{(4)}(\xi)$ if $f \in C^4(a, b)$, $\xi \in [a, b]$

- $f \in C^0(a, b)$ if f is continuous in $[a, b]$ (also denote as $C(a, b)$)
- $f \in C^1(a, b)$ if f and f' are in $C^0(a, b)$ (that is, f and f' are continuous in $[a, b]$)



- $f \in C^n(a, b)$ if $f, f', \dots, f^{(n)}$ are in $C^0(a, b)$

Error estimation (Composite trapz. rule)



$$\mathcal{E} = \frac{(b-a)^3}{12} f''(\varphi)$$

$$\mathcal{E}_i = \frac{h^3}{12} f''(\varphi_i), \quad \varphi_i \in [x_i, x_{i+1}]$$

Comp. Simpson

$$\mathcal{E} = -\frac{(b-a)^5}{180} f^{(4)}(\varphi) h^4$$

$\rightarrow \mathcal{O}(h^4)$

$$\mathcal{E} = \sum_{i=1}^n \mathcal{E}_i = \frac{h^3}{12} \sum_{i=1}^n f''(\varphi_i) \quad (*)$$

$$\varphi \in [a, b]$$

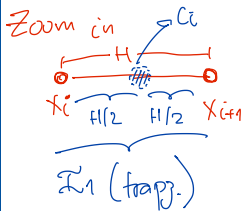
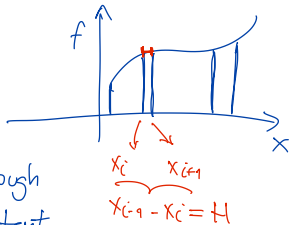
* Generalised mean value theorem: $\sum_{i=1}^n f''(\varphi_i) = n f''(\varphi)$, $f''(\varphi) = \frac{\sum_{i=1}^n f''(\varphi_i)}{n}$

$$\Rightarrow (*) \quad \mathcal{E} = \frac{h^3}{12} n f''(\varphi) = \frac{h^2}{12} (nh) f''(\varphi) = \frac{(b-a)}{12} f''(\varphi) h^2 = \boxed{\mathcal{O}(h^2) \approx \mathcal{E}}$$

Conclusion: the composite trap. rule converges quadratically ($\mathcal{O}(h^2)$)

Error estimation (adaptive trapz.)

$$\mathcal{E} = \frac{(b-a)^3}{12} f''(\xi) \Rightarrow \frac{(x_{i+1} - x_i)^3}{12} f''(\xi_i)$$



* Assumption: H is small enough that f'' is approximately constant.

* \mathcal{I}_1 : quadrature result in $[x_i, x_{i+1}]$

* \mathcal{I}_2 : quadrature results in $[x_i, c_i]$ and $[c_i, x_{i+1}]$ (added)

Error estimates:

$$\begin{aligned} \mathcal{I}_1 - \int_{x_i}^{x_{i+1}} f dx &= \frac{H^3}{12} f'' \approx CH^3 \\ \mathcal{I}_2 - \int_{x_i}^{x_{i+1}} f dx &= 2 \frac{(H/2)^3}{12} f'' \approx \frac{CH^3}{4} \end{aligned}$$

$\mathcal{E}_2 = ?$

(-) Known

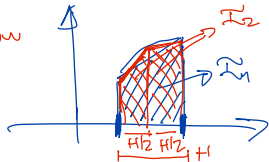
$$\Rightarrow \mathcal{I}_1 - \mathcal{I}_2 \approx \frac{3CH^3}{4}$$

$$\hookrightarrow CH^3 \approx \frac{4}{3} (\mathcal{I}_1 - \mathcal{I}_2)$$

Error estimation

$$E_2 = \mathcal{I}_2 - \int_{x_i}^{x_{i+1}} f dx \approx \frac{1}{4} H^3 \approx \frac{1}{4} \frac{4}{3} (\mathcal{I}_1 - \mathcal{I}_2) = \frac{\mathcal{I}_1 - \mathcal{I}_2}{3} = E_2$$

actual error \rightarrow cannot know in practice



We can compute \rightarrow error estimator because we have \mathcal{I}_2 and \mathcal{I}_1 (results of the quadrature)

* E_2 will be compared to a give tolerance "tol" to determine whether our numerical integral (within $[x_i, x_{i+1}]$) is accurate enough

* Mind that $\int_{x_i}^{x_{i+1}} f dx = \mathcal{I}_2 - E_2 \approx \mathcal{I}_2 - E_2$ that is, we get "for free" an even better approximation for $\int_{x_i}^{x_{i+1}} f dx$ than simply \mathcal{I}_2 .