TDT4127 Programming and Numerics Week 36

Numerical integration

Algorithms: midpoint, trapezoidal and Simpson's rules

Learning goals

- Goals
  - Numerical integration
    - Algorithm statements
    - Error analysis
    - Implementation tips

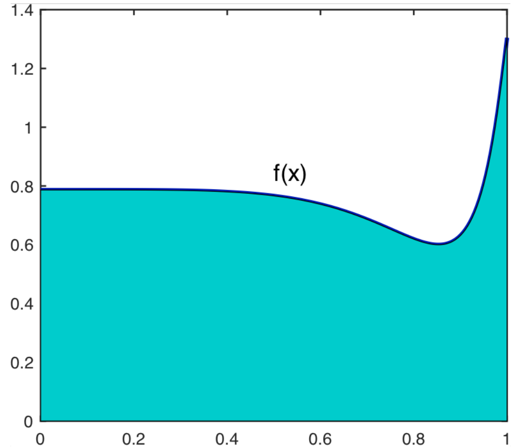
- Curriculum
  - Exercise 3
  - Auditorium exercise 1

Numerical integration

- Everyone loves to integrate! But it can be hard.

$$\int_0^1 \tan(\cos(\sin(\mathrm{e}^{x^5})))\mathrm{d}x = ?$$

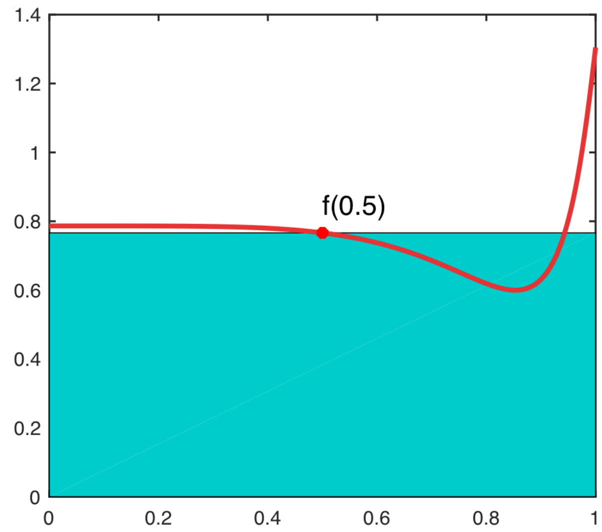
- Integrating in 1D = Finding area under the graph



- The idea: Approximate *f*(*x*) by something easier to integrate
  - In particular, *polynomials* are really easy and approximate well!

Midpoint rule

- Approximate the function by a **constant** and integrate
  - Best constant is the value at the midpoint, $f((a+b)/2)$.

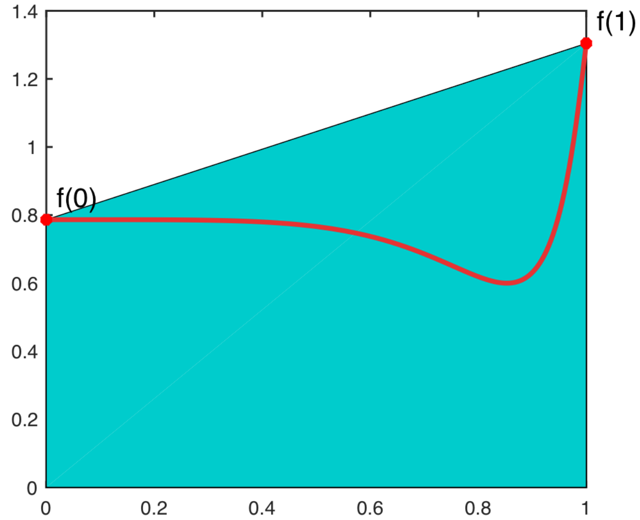


$$\int_a^b f(x)\mathrm{d}x \approx f\left(\frac{a+b}{2}\right)(b-a)$$

Trapezoidal rule

- Approximate the function *f* by a **linear** function *g*
  - Choose *g* to interpolate *f* at the endpoints; $g(a) = f(a)$, $g(b) = f(b)$

$$g(x) = f(a)(x-b)/(a-b) + f(b)(x-a)(b-a)$$

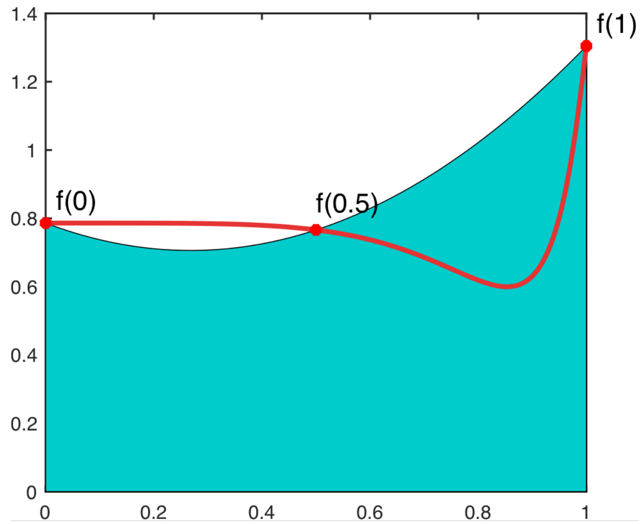


$$\int_a^b f(x)\mathrm{d}x \approx (f(a) + f(b))\,\frac{b-a}{2}$$

Simpson's rule

- Approximate the function *f* by a **quadratic** function *g*
  - Interpolate at c = (a+b)/2; *g*(*a*) = *f*(*a*), *g*(*b*) = *f*(*b*), *g*(*c*) = *f*(*c*)

$$f(x) \approx g(x) = f(a)\frac{(x-b)(x-c)}{(a-b)(a-c)} + f(b)\frac{(x-a)(x-c)}{(b-a)(b-c)} + f(c)\frac{(x-a)(x-b)}{(c-b)(c-b)}.$$



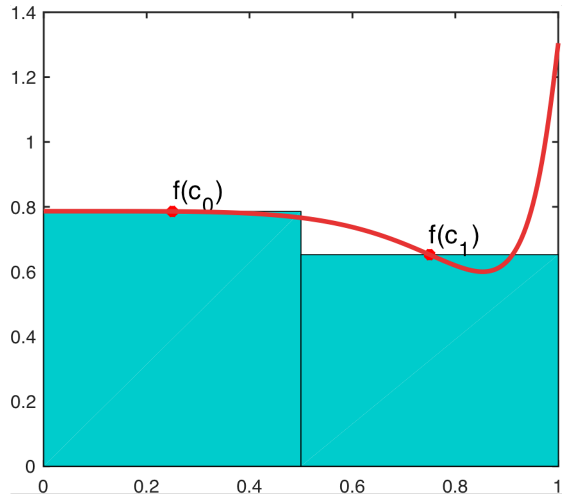
$$\int_a^b f(x)\mathrm{d}x \approx \frac{b-a}{6}\left(f(a) + 4f(c) + f(b)\right).$$

Composite rules

- All three rules give *alright* estimates
  - But we can see with the naked eye that they make mistakes!
- To improve, we split the interval [a,b] into smaller ones
  - Typically, we call the number of intervals N
  - We will consider intervals of fixed width h
    - Other choices exist (leading to Gaussian quadrature)
    - This is not curriculum, but is widely used in practice
  - Splitting an interval of width (b-a) into N parts gives a width of $h=(b-a)/N$.

Composite midpoint rule

- Use a **constant** approximation on each subinterval
  - Subintervals: $[x_k, x_{k+1}]$, $k = 0,\ldots,N-1$. $x_k = a + kh$. $h=(b-a)/N$.



$N = 2$, $h = 0.5$

$$\int_a^b f(x)\mathrm{d}x \approx h \sum_{k=0}^{N-1} f(c_k), \qquad c_k = \frac{x_{k+1} + x_k}{2}$$

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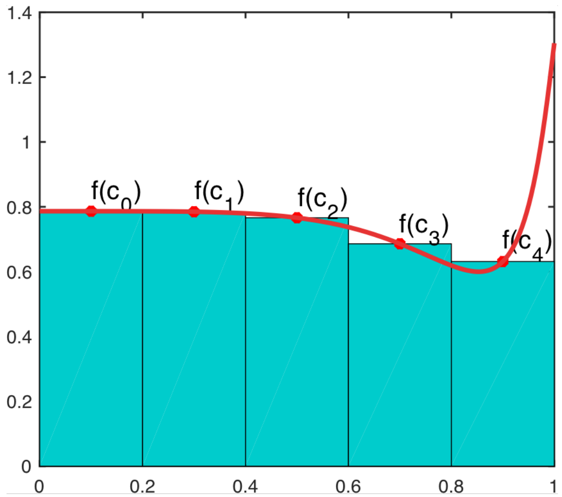

$N = 5$, $h = 0.2$

$$\int_a^b f(x)\mathrm{d}x \approx h \sum_{k=0}^{N-1} f(c_k), \qquad c_k = \frac{x_{k+1} + x_k}{2}$$

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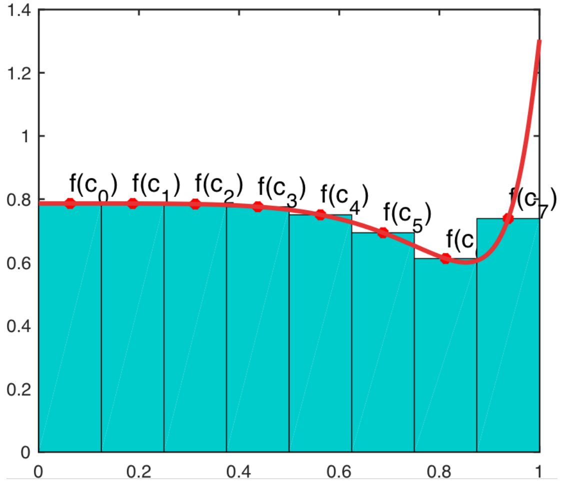

$N = 8$, $h = 0.125$

$$\int_a^b f(x)\mathrm{d}x \approx h \sum_{k=0}^{N-1} f(c_k), \qquad c_k = \frac{x_{k+1} + x_k}{2}$$

Composite trapezoidal rule

- Use a **linear** approximation on each subinterval
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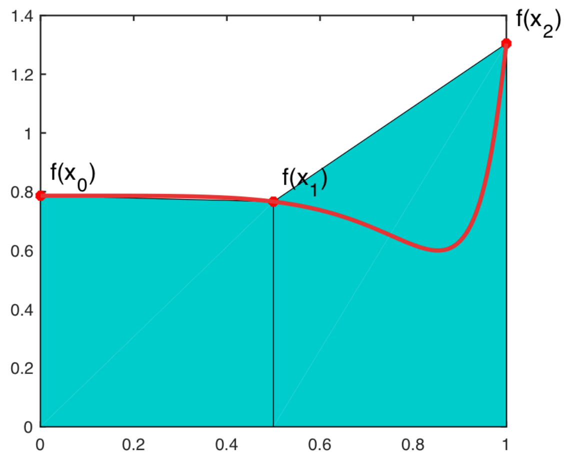

$N = 2$, $h = 0.5$

$$\int_a^b f(x)\mathrm{d}x \approx \frac{h}{2}\left(f(x_0) + 2\sum_{k=0}^{N-1} f(x_1) + f(x_N)\right)$$

Composite trapezoidal rule

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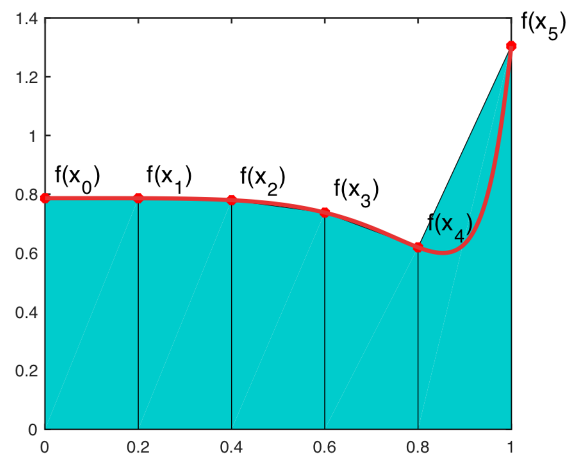

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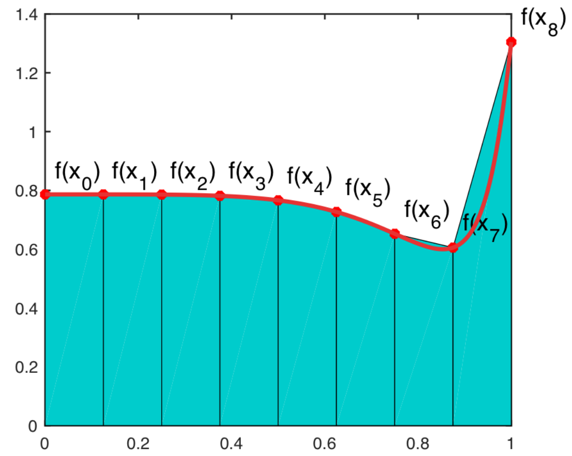

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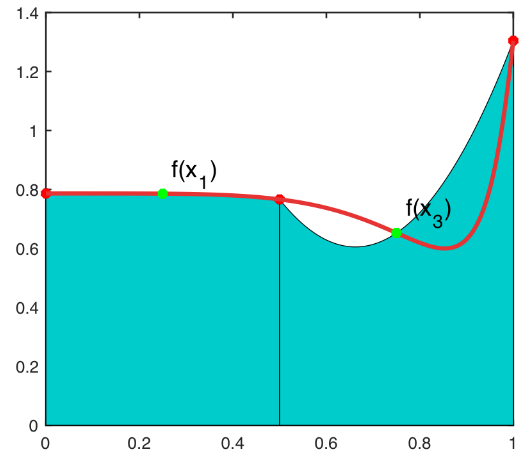
Composite Simpson's rule

- Use a **quadratic** approximation on each subinterval
  - Subintervals: $[x_{2k}, x_{2k+2}]$, $k = 0,\ldots,N-1$. $x_k = a + kh$. $h=(b-a)/2N$.



$N = 2$, $h = 0.5$

$$\int_a^b f(x)\mathrm{d}x \approx \frac{h}{3}\left(f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \ldots + 2f(x_{2N-2}) + 4f(x_{2N-1}) + f(x_{2N})\right), \qquad h = \frac{b-a}{2N}$$

Composite Simpson's rule

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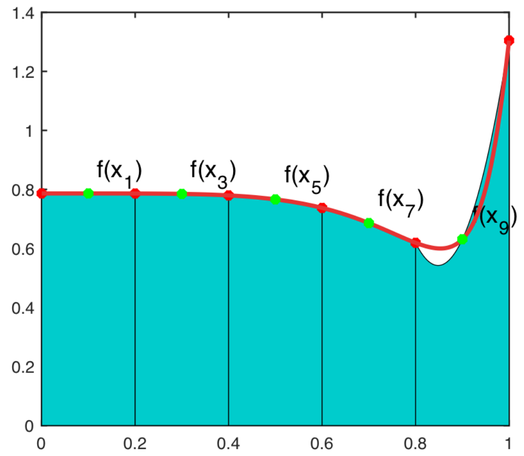

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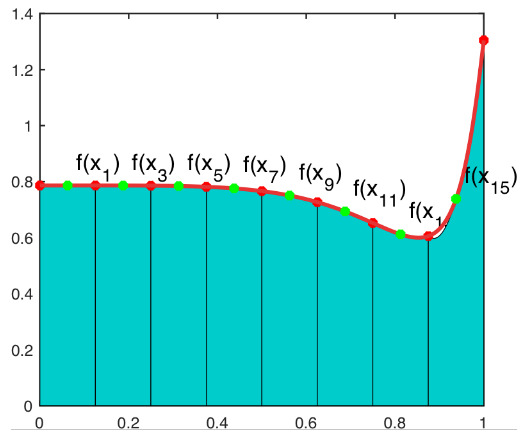

$N = 8$, $h = 0.125$

$$\int_a^b f(x)\mathrm{d}x \approx \frac{h}{3}\left(f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \ldots + 2f(x_{2N-2}) + 4f(x_{2N-1}) + f(x_{2N})\right), \qquad h = \frac{b-a}{2N}$$

  - Note the odd/even coefficients of 4 and 2

Error analysis

- We can get an estimate for the error of the midpoint method assuming f is *continuously differentiable* (also written C^1)
  - A function f is continuously diff'ble if f' is continuous.
  - Examples: $f(x) = x^2$ and $f(x) = e^x$
  - Non-example: $f(x) = |x|$
- The midpoint rule has an error estimate:

$$E_{\mathrm{MP}} = \left| \int_a^b f(x)\mathrm{d}x - (b-a) f\left(\frac{a+b}{2}\right) \right| \leq \frac{(b-a)^3}{24} M$$

- Where M is the maximum value of $|f''(x)|$ on $[a,b]$.
  - *Note that this estimate requires continuous differentiability of* f

Error analysis

- For the composite midpoint method, we simply use the error estimate on each subinterval [x_k, x_{k+1}]

$$E_{\mathrm{MP},k} = \left| \int_{x_k}^{x_{k+1}} f(x)\mathrm{d}x - hf\left(c_k\right) \right| \leq \frac{h^3}{24}M$$

- Summing up all of these, we find the total error

$$E_{\mathrm{CMP}} \leq \sum_{k=0}^{N-1} E_{\mathrm{MP},k} \leq \sum_{k=0}^{N-1} \frac{h^3}{24}M = N\frac{h^3}{24}M = \frac{(b-a)^3}{24N^2}M$$

- As N increases, the error decreases and so the approximation converges to the true integral as $N \rightarrow \infty$

Error analysis

- Similar estimates can be made for (composite) trapezoidal (TR) and (composite) Simpson's (SI) rules

$$E_{\mathrm{TR}} = \left| \int_a^b f(x)\mathrm{d}x - \frac{b-a}{2}(f(a)+f(b)) \right| \leq \frac{(b-a)^3}{12} M$$

$$E_{\mathrm{CTR}} \leq \frac{(b-a)^3}{12N^2} M$$

$$E_{\mathrm{SI}} = \left| \int_a^b f(x)\mathrm{d}x - \frac{b-a}{6}\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right) \right| \leq \frac{(b-a)^5}{2880} M_4$$

$$E_{\mathrm{CSI}} \leq \frac{(b-a)^5}{2880N^4} M_4, \qquad M_4 = |\max_{a \leq x \leq b} f''''(x)|$$

- Note that composite Simpson goes as $1/N^4$
  - And requires a continuous 4th derivative of f, (Notation: f is C^4).

Guaranteed error estimates

- The error analysis is useful since it gives us the worst-case behaviour of the algorithm
- If we want, we can guarantee a level of precision in the numerical approximation
  - For example, to make sure the integral of a C^4 function has error at most ε, use the Simpson's rule and choose N such that

$$E_{\text{CSI}} \leq \frac{(b-a)^5}{2880N^4} M_4 = \epsilon, \qquad M_4 = |\max_{a \leq x \leq b} f''''(x)|$$

  - Note: the estimates may be too conservative, suggesting more iterations than necessary, but they are safe

Implementation

- Sums and for loops go hand in hand
- Example:

$$S = \sum_{k=0}^{N} a_k$$

<u>Translation into code:</u>

```
S = 0
for k in range(0,N+1)
    a_k = …
    S = S + a_k
```

Summary

- Numerical integration is used to evaluate integrals
- We have seen three methods
  - Midpoint rule, trapezoidal rule and Simpson’s rule
- Also seen the composite rules based on these
  - With error analysis, useful for guaranteeing errors!

Questions?