

# Calculus and Differential Equations I

MATH 250 A

## Numerical approximations

## Numerical approximation of definite integrals

- You should already be familiar with the **left and right-hand Riemann sums** used in the definition of the definite integral:

$$I \equiv \int_a^b f(x) dx = \lim_{n \rightarrow \infty} \sum_{i=0}^{n-1} f(x_i) \Delta x = \lim_{n \rightarrow \infty} \sum_{i=1}^n f(x_i) \Delta x,$$

where  $\Delta x = (b - a)/n$  and  $x_i = a + i \Delta x$ .

- The **left and right rules** respectively approximate the integral  $I$  with  $\text{LEFT}(n)$  and  $\text{RIGHT}(n)$ , where

$$\text{LEFT}(n) = \sum_{i=0}^{n-1} f(x_i) \Delta x, \quad \text{RIGHT}(n) = \sum_{i=1}^n f(x_i) \Delta x,$$

with  $\Delta x$  and  $x_i$  defined as above.

[▶ Link to Geogebra](#)

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## Numerical approximation of definite integrals (continued)

- The **midpoint rule** consists in approximating the definite integral by evaluating  $f$  at the midpoint between  $x_i$  and  $x_{i+1}$ :

$$\text{MID}(n) = \sum_{i=0}^{n-1} f\left(\frac{x_i + x_{i+1}}{2}\right) \Delta x.$$

- The **trapezoid rule** approximates the area under the graph of  $f$  between  $x_i$  and  $x_{i+1}$  with the area of the corresponding trapezoid:

$$\text{TRAP}(n) = \sum_{i=0}^{n-1} \left( \frac{f(x_i) + f(x_{i+1})}{2} \right) \Delta x.$$

- From the above formula, one can see that

$$\text{TRAP}(n) = \frac{1}{2} (\text{LEFT}(n) + \text{RIGHT}(n)).$$

## Overestimates and underestimates

- Assume that  $f$  is increasing between  $a$  and  $b$  and that we approximate  $I = \int_a^b f(x) dx$  with  $\text{LEFT}(n)$ . Which of the following statements is correct?

- $\text{LEFT}(n)$  is an underestimate
- $\text{LEFT}(n)$  is an overestimate
- $\text{LEFT}(n)$  is exact

- If  $f$  is increasing on  $[a, b]$ , then

$$\text{LEFT}(n) \leq \int_a^b f(x) dx \leq \text{RIGHT}(n).$$

- Similarly, if  $f$  is decreasing on  $[a, b]$ , then

$$\text{RIGHT}(n) \leq \int_a^b f(x) dx \leq \text{LEFT}(n).$$

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## Overestimates and underestimates (continued)

- In order to ensure that  $\text{TRAP}(n)$  is an **overestimate**, which of the following requirements do we need?

- 1  $f$  is increasing
- 2  $f$  is concave up
- 3  $f$  is concave down
- 4  $f$  is decreasing

- If  $f$  is **concave up** on  $[a, b]$ , then

$$\text{MID}(n) \leq \int_a^b f(x) dx \leq \text{TRAP}(n).$$

- Similarly, if  $f$  is **concave down** on  $[a, b]$ , then

$$\text{TRAP}(n) \leq \int_a^b f(x) dx \leq \text{MID}(n).$$

## Example of application

- Assume that the function  $f$  is **positive, decreasing, and concave down** on  $[a, b]$ . Let  $I = \int_a^b f(x) dx$ .
- Assume that the values of  $\text{LEFT}(10)$ ,  $\text{RIGHT}(10)$ ,  $\text{TRAP}(10)$ , and  $\text{MID}(10)$  are, **in random order**, given by

0.703, 0.724, 0.735, 0.745.

- Use the above to assign a value to each of  $\text{LEFT}(10)$ ,  $\text{RIGHT}(10)$ ,  $\text{TRAP}(10)$ , and  $\text{MID}(10)$ .
- Then, indicate which of the statements below is correct:
  - 1  $0.703 \leq I \leq 0.724$
  - 2  $0.724 \leq I \leq 0.735$
  - 3  $0.735 \leq I \leq 0.745$

## Approximation errors

- If we use a numerical method, say the left rule, to approximate a definite integral  $I$ , we define the **absolute error**  $E_L(n)$ , as

$$E_L(n) = I - \text{LEFT}(n).$$

- One can show that  $|E_L(n)|$  and  $|E_R(n)|$  are **linear functions of  $1/n$** .
- Similarly,  $|E_T(n)|$  and  $|E_M(n)|$  decrease **quadratically** as  $n$  is increased.
- This can be improved by using **Simpson's rule**, given by

$$\text{SIMP}(n) = \frac{1}{3} (2\text{MID}(n) + \text{TRAP}(n)).$$

- One can show that the error  $|E_S(n)|$  decreases **like  $1/n^4$** .

## Numerical integration of ODEs

$$\frac{dy}{dx} = g(x, y)$$

- The above differential equation may formally be integrated as

$$y(x+h) - y(x) = \int_x^{x+h} g(t, y(t)) dt.$$

- If we know  $y(x)$ , a **numerical approximation** of  $y(x+h)$  may thus be obtained by finding an estimate of the integral in the right-hand-side of the above equation.
- **Euler's method** consists in assuming that  $g(t, y(t))$  is constant on the interval  $[x, x+h]$ , and equal to  $g(x, y(x))$ , where  $x$  is the **left end-point** of the interval.
- We thus have

$$y(x+h) \simeq y(x) + hg(x, y(x)).$$

## Numerical integration of ODEs (continued)

$$\frac{dy}{dx} = g(x, y)$$

- If we use the **midpoint rule**, then we obtain the **modified Euler method** mentioned in the lab,

$$y(x+h) \simeq y(x) + h g\left(x + \frac{h}{2}, y(x) + \frac{h}{2} g(x, y(x))\right).$$

- If we use the **trapezoid rule**, we obtain **Heun's method** (sometimes also called improved Euler's method)

$$y(x+h) \simeq y(x) + \frac{h}{2} (g(x, y(x)) + g(x+h, y(x) + hg(x, y(x))))).$$

## Numerical error

- **Numerical simulations** are very powerful tools, but if we want to trust their predictions, it is essential to know their limitations. In particular, we need to be able to **understand and control numerical errors**.
- All of the above methods are susceptible to **two types of error**:

- 1 The **discretization error** is due to approximation errors in the numerical method.
- 2 The **round-off error** is due to the fact that a computer does not perform exact calculations.

For instance, in MATLAB, `eps` returns "the distance from 1.0 to the next largest double-precision number".

## Discretization error

The **discretization error** has two sources:

- 1 The **local discretization error**  $e_n$ , which is the error made at each time step due to the fact that we approximate an integral on the right-hand side of the equation:

$$e_n = \tilde{y}_n - y(x_n),$$

where  $y(x_n)$  is the exact solution, and  $\tilde{y}_n$  is the numerical approximation of  $y(x_n)$  assuming that  $y(x_{n-1})$  is known exactly.

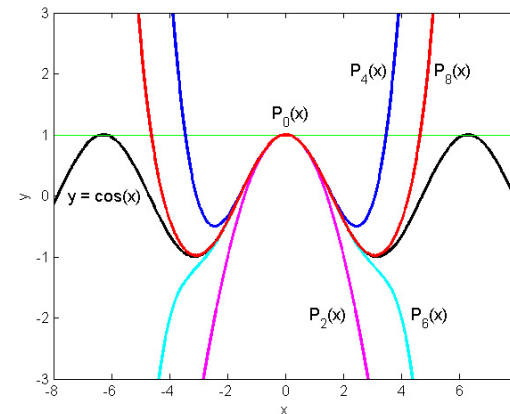
- 2 The **global discretization error**  $E_n$ , which is the error made on  $y(x_n)$  when it is evaluated from an initial condition  $y_0$  after  $n$  numerical integration steps:

$$E_n = y_n - y(x_n),$$

where  $y_n$  is the numerical solution obtained after  $n$  steps.

## Taylor polynomials

We now turn to the question of approximating a function of one variable by polynomials.



The **Taylor polynomial** of degree  $n$  of the function  $f$  near  $x = a$  is a polynomial that matches the value of  $f$  and of its first  $n$  derivatives at the point  $x = a$ .

The figure above shows the graph of  $\cos(x)$  and of the Taylor polynomials of degree up to 8 near  $x = 0$ .

## Taylor polynomials (continued)

- The **Taylor polynomial** of degree  $n$ , centered at  $x = a$ , of a function  $f$  is given by

$$P_n(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}f''(a) + \dots + \frac{(x-a)^n}{n!}f^{(n)}(a).$$

- Of course, the above assumes that  $f$  has at least  $n$  times differentiable near  $a$ . In what follows, we assume that  $f$  is smooth, for simplicity.
- One can show that the **error** made by replacing  $f$  by its Taylor polynomial of degree  $n$  is given by

$$f(x) = P_n(x) + R_n(x), \quad R_n(x) = \frac{(x-a)^{n+1}}{(n+1)!}f^{(n+1)}(\xi),$$

where  $\xi \in (a, x)$ .

[▶ Link to d'Arbeloff Taylor Polynomials software](#)

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## Numerical approximation of definite integrals revisited

$$\int_a^b f(x) dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x) dx, \quad x_i = a + i\Delta x, \quad \Delta x = \frac{b-a}{n}.$$

- For the **left rule**, for each  $x \in [x_i, x_{i+1}]$ , we have

$$f(x) = f(x_i) + (x-x_i)f'(\xi(x)), \quad \xi(x) \in (x_i, x).$$

- From this formula, we see that if  $f'$  is **positive** and bounded by  $M$  between  $x_i$  and  $x_{i+1}$ , then

$$0 \leq f(x) - f(x_i) \leq M(x-x_i),$$

which gives that **LEFT is an underestimate** and

$$\left| \int_{x_i}^{x_{i+1}} f(x) dx - f(x_i) \Delta x \right| \leq \int_{x_i}^{x_{i+1}} M(x-x_i) dx = M \frac{(\Delta x)^2}{2}.$$

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## Approximation errors

- For the **midpoint rule**, we have, with  $m = \frac{x_i + x_{i+1}}{2}$ ,

$$f(x) = f(m) + (m-x)f'(m) + \frac{1}{2}(x-m)^2 f''(\xi(x)), \quad \xi(x) \in (x_i, x).$$

- We can check that

$$\int_{x_i}^{x_{i+1}} (f(m) + (m-x)f'(m)) dx = f(m) \Delta x,$$

so that if  $f''$  is **positive** and bounded by  $M$  between  $x_i$  and  $x_{i+1}$ , then

$$0 \leq f(x) - [f(m) + (m-x)f'(m)] \leq \frac{M}{2}(x-m)^2,$$

which gives that **MID is an underestimate** and that the larger  $|f''|$ , the larger the error.

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## Approximation errors (continued)

- Finally, for the **trapezoid rule**, we have (by integration by parts)

$$\int_{x_i}^{x_{i+1}} f(x) dx = [(x-m)f(x)]_{x_i}^{x_{i+1}} - \int_{x_i}^{x_{i+1}} (x-m)f'(x) dx.$$

- We can use a Taylor expansion for  $f'(x)$  near  $x = m$  to see that if  $f''$  is **positive** between  $x_i$  and  $x_{i+1}$ , then **TRAP gives an overestimate**.
- Moreover, the error over an interval of length  $\Delta x$  is bounded by  $M(\Delta x)^3/12$ , where  $M$  is the maximum of  $|f''|$  over that interval.
- For all of these methods, if the error on the integral between  $x_i$  and  $x_{i+1}$  is of order  $(\Delta x)^{p+1}$ , then **the error on the integral between  $a$  and  $b$  is of order  $1/n^p$** , where  $n$  is the number of sub-intervals.

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## Numerical integration of ODEs revisited

- A numerical method is **consistent** if the local discretization error goes to zero as  $h \rightarrow 0$ .
- A numerical method is **convergent** if the global discretization error goes to zero as  $h \rightarrow 0$ .
- Typically, one uses Taylor expansions to decide whether a numerical method is consistent and convergent.
- A numerical method may also be **unstable**, in the sense that a numerical solution to  $y' = \lambda y$  with  $\lambda < 0$  can display growth.
- These are topics typically discussed in an **introductory course on numerical analysis**, such as MATH 475.
- Finally, one should keep in mind that a numerical method is a **map** of the form  $y_{n+1} = G(y_n, n)$ , and that if  $G$  is nonlinear, chaos may be observed.

[▶ Link to Chaos on the Web](#)