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:

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

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

- The left and right rules respectively approximate the integral I with LEFT(n) and RIGHT(n), where

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

with Δx and x_i defined as above.

Link to Geogebra

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

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

Overestimates and underestimates

1. Assume that f is increasing between a and b and that we approximate $I = \int_a^b f(x)\,dx$ with LEFT(n). Which of the following statements is correct?
   1. LEFT(n) is an underestimate
   2. LEFT(n) is an overestimate
   3. LEFT(n) is exact
2. If f is increasing on $[a, b]$, then

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

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

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

Overestimates and underestimates (continued)

- In order to ensure that 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 LEFT(10), RIGHT(10), TRAP(10), and 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 LEFT(10), RIGHT(10), TRAP(10), and 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

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

- 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

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

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)

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

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.

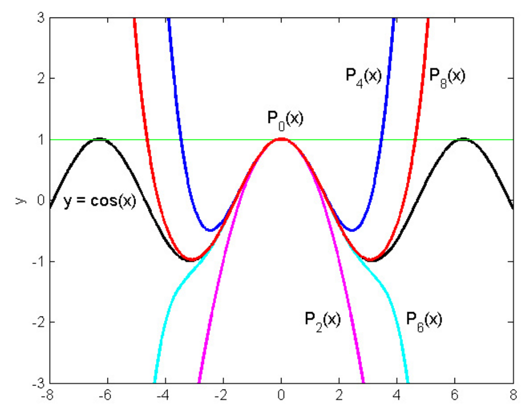
2. The global discretization error E_n, which is the error made on $y(x_n)$ when it is evaluated from an initial condition y_0 after n numerical integration steps:

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

   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

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

- Of course, the above assumes that f has is 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

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

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

Link to d'Arbeloff Taylor Polynomials software

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

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

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

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

which gives that LEFT is an underestimate and

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

Approximation errors

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

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

- We can check that

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

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

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

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

Approximation errors (continued)

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

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

- 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 Δx 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.

Numerical integration of ODEs revisited

- A numerical method is consistent if the local discretization error goes to zero as $h \to 0$.
- A numerical method is convergent if the global discretization error goes to zero as $h \to 0$.
- 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