

FALL 2024

MEETING #2

Computational Modeling in Engineering and the Sciences
Computer Science Undergraduate Directed Reading Program

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AGENDA

- Discussion
- Introduction to ODEs in 1D
- Demo: programming explicit Euler

Assignment: Find a paper discussing high-order integration methods for ordinary differential equations, e.g., Runge-Kutta, Adams-Bashforth, &c. Look for the motivation, advantages, disadvantages, and broader context of the method.

Discussion: Research applications of “computational modeling” and find an interesting example to tell us about.

ORDINARY DIFFERENTIAL EQUATION(S)

ordinary differential equation

a differential equation with only one **independent** variable

Introducing the IVP:

$$\frac{dx}{dt} = f(x, t)$$

$$x(t_0) = x_0$$

$$x(t) = ?$$

ORDINARY DIFFERENTIAL EQUATION(S)

Reintroducing a thing from Calculus that you probably never thought you would use again in your life

Lagrange Polynomials are very helpful to derive and evaluate derivative approximations.

E.g., a polynomial approximating $x(t)$ centered at $t = \tau$

The n th derivative of this polynomial is exact at τ and is usually a reasonable guesstimate in the neighborhood.

$$x(t) \approx \ell_{\tau}(t) = x(\tau) + \frac{dx}{dt} \Big|_{\tau} (t - \tau) + \frac{1}{2} \frac{d^2x}{dt^2} \Big|_{\tau} (t - \tau)^2 + \frac{1}{3!} \frac{d^3x}{dt^3} \Big|_{\tau} (t - \tau)^3 \\ + \dots + \frac{1}{n!} \frac{d^n x}{dt^n} \Big|_{\tau} (t - \tau)^n + \dots$$

ORDINARY DIFFERENTIAL EQUATION(S)

Deriving integration methods from finite differences

We can use the definition of a derivative to make some fudgy approximations.

$$\begin{aligned}\frac{dx}{dt} \Big|_t &:= \lim_{h \rightarrow 0} \frac{x(t+h) - x(t)}{h} \\ &= \lim_{h \rightarrow 0} \frac{x(t) - x(t-h)}{h} \\ &= \lim_{h \rightarrow 0} \frac{x(t+h) - x(t-h)}{2h}\end{aligned}$$

ORDINARY DIFFERENTIAL EQUATION(S)

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$$\begin{aligned}\frac{dx}{dt} \Big|_t &:= \lim_{h \rightarrow 0} \frac{x(t+h) - x(t)}{h} &= \frac{x(t+h) - x(t)}{h} + \mathcal{O}(h) \\ &= \lim_{h \rightarrow 0} \frac{x(t) - x(t-h)}{h} &= \frac{x(t) - x(t-h)}{h} + \mathcal{O}(h) \\ &= \lim_{h \rightarrow 0} \frac{x(t+h) - x(t-h)}{2h} &= \frac{x(t+h) - x(t-h)}{2h} + \mathcal{O}(h^2)\end{aligned}$$

Forward Euler method

ORDINARY DIFFERENTIAL EQUATION(S)

$$\left. \frac{dx}{dt} \right|_t \approx \frac{x(t + \Delta t) - x(t)}{\Delta t}$$

$$x(t + \Delta t) = x(t) + \Delta t f(x(t), t)$$

$$x_{n+1} = x_n + \Delta t f(x_n, t_n)$$

Backward Euler method

ORDINARY DIFFERENTIAL EQUATION(S)

$$\left. \frac{dx}{dt} \right|_t \approx \frac{x(t) - x(t - \Delta t)}{\Delta t}$$

$$x(t) = x(t - \Delta t) + \Delta t f(x(t), t)$$

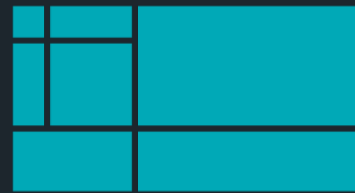
$$x_{n+1} = x_n + \Delta t f(x_{n+1}, t_{n+1})$$

DEMO: PROGRAMMING EXPLICIT EULER

Demo time!

$$\frac{dx}{dt} = -\alpha x, \quad \alpha > 0$$

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