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FOR COMPUTATIONAL ENGINEERING & SCIENCES

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.

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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:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x,t)$$
$$x(t_0) = x_0$$
$$x(t) = ?$$

ORDINARY DIFFERENTIAL EQUATION(S)

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

Taylor Series are very helpful to derive and evaluate derivative approximations.

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

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

$$x(t) \approx p_\tau(t) = x(\tau) + \left.\frac{\mathrm{d}x}{\mathrm{d}t}\right|_\tau (t-\tau) + \frac{1}{2}\left.\frac{\mathrm{d}^2x}{\mathrm{d}t^2}\right|_\tau (t-\tau)^2 + \frac{1}{3!}\left.\frac{\mathrm{d}^3x}{\mathrm{d}t^3}\right|_\tau (t-\tau)^3$$
$$+ \ldots + \frac{1}{n!}\left.\frac{\mathrm{d}^nx}{\mathrm{d}t^n}\right|_\tau (t-\tau)^n + \ldots$$

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ORDINARY DIFFERENTIAL EQUATION(S)

Deriving integration methods from finite differences

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

$$
\begin{aligned}
\left.\frac{\mathrm{d}x}{\mathrm{d}t}\right|_t &:= \lim_{h\to 0}\frac{x(t+h)-x(t)}{h}\\
&= \lim_{h\to 0}\frac{x(t)-x(t-h)}{h}\\
&= \lim_{h\to 0}\frac{x(t+h)-x(t-h)}{2h}
\end{aligned}
$$

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= \lim_{h\to 0}\frac{x(t)-x(t-h)}{h} \qquad &= \frac{x(t)-x(t-h)}{h} + \mathcal{O}(h) \\
= \lim_{h\to 0}\frac{x(t+h)-x(t-h)}{2h} \qquad &= \frac{x(t+h)-x(t-h)}{2h} + \mathcal{O}(h^2)
\end{aligned}
$$

ORDINARY DIFFERENTIAL EQUATION(S)

Forward Euler method

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

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

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

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ORDINARY DIFFERENTIAL EQUATION(S)

Backward Euler method

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

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

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

DEMO: PROGRAMMING EXPLICIT EULER

Demo time!

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\alpha x, \quad \alpha > 0$$

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