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FOR COMPUTATIONAL ENGINEERING & SCIENCES

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MEETING #2

Computational Modeling in Engineering and the Sciences

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AGENDA

- Discussion of Konstantinovsky - Mastering the SEIR Model
- Introduction to ODEs
- Demo: ODEs in 1D

Assignment: Read first chapter of Baigent - Lotka-Volterra Dynamics. We'll discuss next week.

Discussion of Konstantinovsky

Introduction to ODEs

Introducing ODEs

- **ordinary differential equation:** a differential equation with only one **independent** variable
- Introducing the IVP:

$$\frac{\mathrm{d}u}{\mathrm{d}t} = f(x, t)$$

$$u(t_0) = u_0$$

$$u(t) = ?$$

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Introducing ODEs

Reintroducing a thing from Calculus you probably thought you would never see 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.

$$u(t) \approx p_\tau(t) = u(\tau) + \frac{\mathrm{d}u}{\mathrm{d}t}\Big|_\tau (t-\tau) + \frac{1}{2}\frac{\mathrm{d}^2u}{\mathrm{d}t^2}\Big|_\tau (t-\tau)^2 + \frac{1}{3!}\frac{\mathrm{d}^3u}{\mathrm{d}t^3}\Big|_\tau (t-\tau)^3$$
$$+ \ldots + \frac{1}{n!}\frac{\mathrm{d}^nu}{\mathrm{d}t^n}\Big|_\tau (t-\tau)^n + \ldots$$

Introducing ODEs

Deriving integration methods from finite differences

- Limit definitions of derivative are good place to start
  - What if h is small?
- Elaborate schemes are less intuitive, but when in doubt…

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

Introducing ODEs

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$$
\begin{aligned}
\left.\frac{\mathrm{d}u}{\mathrm{d}t}\right|_{\tau} &:= \lim_{h\to 0}\frac{u(\tau+h)-u(\tau)}{h} && = \frac{u(\tau+h)-u(\tau)}{h} + \mathcal{O}(h) \\
&= \lim_{h\to 0}\frac{u(\tau)-u(\tau-h)}{h} && = \frac{u(\tau)-u(\tau-h)}{h} + \mathcal{O}(h) \\
&= \lim_{h\to 0}\frac{u(\tau+h)-u(\tau-h)}{2h} && = \frac{u(\tau+h)-u(\tau-h)}{2h} + \mathcal{O}(h^2)
\end{aligned}
$$

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Introducing ODEs

Deriving integration methods from finite differences

- Forward Euler method

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

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

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

Introducing ODEs

Deriving integration methods from finite differences

- 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: ODEs in 1D

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

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