Intro to SciML: forward problems

"AI" and "data-driven" nearly synonymous

ML = Machine Learning

Motivation for the course is to not duplicate CS courses
- we won't do NLP or LLM, not much computer vision
  - Some overlap w/ scientific imaging
- look at data-driven methods
  (and their advantages/disadvantages)
  for scientific applications.

Simplifying, here are broad classes of problems we'll attack:

① **Forward Problems**   eg physical simulation,   especially multiphysics + high dim.
Solving diff. eq'n ...   Stochastic D.E. in finance

  Ex: Climate modeling
    multiphysics, multiscale
    Even just fluid flow (Navier Stokes Eq.)
      - Ideally solve N-S via "Direct Numerical Simulation" (DNS)
        on a very fine space-time grid.
        Completely impossible!
                Air flow over air foil for 1 ms: barely possible
                Whole Earth for 100 years: no way

        - DNS at coarse resolution?
            Bad idea. Under-resolved scales still
            have systematic contribution to large scale
                eg. energy isn't conserved, etc.

We'll study the subtle issues that pure ML papers Sometimes miss

        - Simplified physical models,
            "LES" or "RANS"   Large Eddy Simulation.
            Don't resolve finest scales but
            try to account for their aggregate effect.
                "closure modeling"
                → use ML here to augment/complement classical model

Or, pure end-to-end ML

Intro to SciML: inverse problems

② Inverse Problems

  Ex: Full Waveform Inversion (FWI)

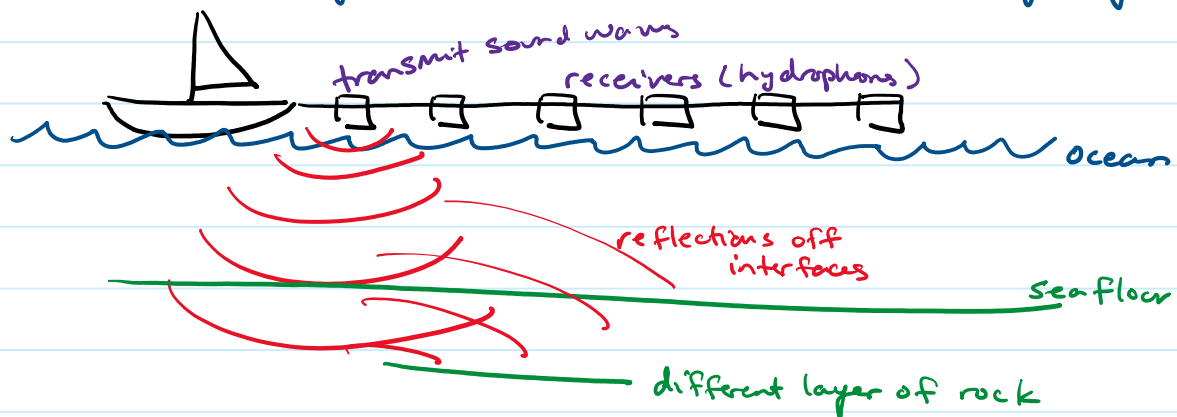 1D wave eq'n (PDE): $u_{tt} = c^2 u_{xx}$, 1D easy to solve

  $u_t = \frac{\partial u}{\partial t}$, $u_{tt} = \frac{\partial^2 u}{\partial t^2}$ etc.

  u = displacement/pressure $u(x,t)$
  c = speed of sound in medium

  Given parameters (like c), initial conditions ("IC")
  and appropriate boundary conditions ("BC"),
  "solving" for u (numerically) is the forward problem
  (eq'n → sol'n)

  Science problem: what's inside something?

  Medical imaging, finding cracks in concrete, geophysics

  transmit sound waves   receivers (hydrophones)
  ocean
  reflections off interfaces
  seafloor
  different layer of rock

  Now, we measure u
      data $\{ u(x_i, t_i) \}_{i=1}^{n}$

  $u_{tt} = c(x)^2 \cdot u_{xx}$ Variable speed of sound

  inverse problem: what is the (parameters of the) equation?
      (sol'n → eq'n)

  Difficult! usually ill-posed, underdetermined.

  Regularize, impose prior information ← great place for ML

                                        try to
      ML can augment or replace classical ideas