SciML - Applications and Cases Studies

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Program

1. Applications of scientific machine learning
   (a) Fluid dynamics
   (b) Materials science
   (c) Biology
   (d) Medicine
   (e) The challenges of applying scientific machine learning to different scientific domains

2. Case studies in scientific machine learning
   (a) Solving partial differential equations with neural networks
   (b) Predicting protein structures with deep learning
   (c) Diagnosing diseases with machine learning
   (d) Epidemiology with machine learning
   (e) The use of case studies to illustrate the power of scientific machine learning
   (f) The challenges of applying scientific machine learning to real-world problems

APPLICATIONS

Applications in Fluid Dynamics

- Laminar flows
- Turbulent flows
- Viscoelastic flows
- Geofluid flows: groundwater, porous media, solute transport
- Biomedical flows
- Aerodynamics
- NWP

Applications in Solid Mechanics

- accelerating simulations: aortic wall stress, material modeling, stresses and cracks
- topology optimization:
- structural analysis
- elastostatics: forward and inverse problems
- additive manufacturing

Applications in Material Science

ML methods are able to

- (1) automate materials' characterization processes and effectively analyze the characterization dataset
- (2) quickly screen the vast material design space (e.g., reducing the prediction time of DFT from 10^3s to 10^{-2} s)
- (3) realize property prediction in complex material systems with limited first-principles understanding
- (4) directly map high-dimensional synthesis recipes to materials with desired properties
- (5) extract generalizable scientific principles from various material systems.

Applications

- Li-ion battery design and manufacturing
- Photovoltaic optimization
- and many, many others...

Applications in Epidemiology

- COVID,
- Anthrax,
- HIV,
- Zika,
- Smallpox,
- Tuberculosis,
- Pneumonia,
- Ebola,
- Dengue,
- Polio,

- Measles.

Applications in Medecine

- Many imaging-related diagnostics

  $\Rightarrow$ cancer tumors
  $\Rightarrow$ glaucomas and retinopathy diagnostics

- Risks of drugs

- Drug design

- Genomic analysis for neurological diseases

- and many, many others...

CASE STUDIES

Solving PDEs

- There is a vast panoply of toolboxes and approaches available.
- They can solve arbitrarily complex models, and they can even find the model itself.
- Once trained, they provide lightning-fast surrogates.

Predicting protein structures

- Predicting the 3D structure of proteins is one of the fundamental grand challenges in biology.

- By solving this challenge, we can dramatically deepen our understanding of human health, disease, and our environment, especially within areas like drug design and sustainability.

  $\Rightarrow$ AlphaFold, a state-of-the-art AI system developed by DeepMind, is able to computationally predict protein structures with unprecedented accuracy and speed

  $\Rightarrow$ It predicts a protein's 3D structure from its amino acid sequence.

  $\Rightarrow$ AlphaFold DB provides open access to over 200 million protein structure predictions to accelerate scientific research.

Diagnosing diseases with Scientific machine learning

- ML has been successfully applied in the healthcare domain to diagnosing diseases.
- The ML techniques have not only been able to diagnose common diseases but are also equally capable of diagnosing rare diseases.
- See next slide for more.

Epidemiology with Scientific machine learning

- ML can be employed to study complex interactions between different biological systems, such as signaling pathways and metabolic networks, to advance our understanding of various biological phenomena and improve the diagnosis and treatment of diseases. These technologies have the potential to significantly impact biological research in a variety of areas, including infectious diseases and epidemiology.

- ML can be used to analyze large datasets, such as genomic data, to identify patterns and trends relevant to the understanding and treatment of infectious diseases

- ML can be employed to predict the likelihood of certain outcomes, such as the spread of a disease, based on historical data and by analyzing datasets generated by epidemiological studies. This can aid epidemiologists in preventing or mitigating outbreaks of infectious diseases, such as influenza and HIV.

- AI can also be utilized to build predictive models that help researchers understand the relationships between different variables, such as gene expression and disease risk, interactions between pathogens and host organisms at the molecular level, and complex molecular interactions within biomolecules.

- ChatGPT can provide the definitions of scientific terms, generate prevalence and risk factor maps of any disease, and so on.

- For epidemiological analysis, using a compartment model, the classical PINN approach can be applied.

  $\Rightarrow$ In DINN [Shaier, Raissi, Seshaiyer. Letters in Biomechanics, 8 (1), 2022], the method is applied to a large number of infectious diseases.

- DA techniques have been applied, in the form of Kalman filter variants, to analyze and predict epidemic spreading.

Bibliography

References

[1] M. Asch. *Digital Twins: from Model-Based to Data-Driven.* SIAM, 2022.