Neural Networks for PDEs Reading Group

CNA + MLD Working Group F2024

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Goals:

- Educate students and faculty in both MLD and mathematics about the emerging interface between machine learning and computational mathematics.
- Fuse expertise in the mathematics department with expertise in the machine learning department to establish collaboration and communication.
- Identify scientific and mathematical problems that are challenging to solve with more traditional techniques from numerical analysis but which we may be able to solve with novel machine learning methods.
- Garner graduate student interest in these problems, leading to downstream projects and publications joint between MLD and mathematics students.

Structure:

- Single 1.5 hour meeting each week.
- Group collectively reads one or two papers each week.
- One attendee takes the lead on presenting, ideally in the form of a chalk talk (with some backup slides for visualization) for one hour.
- Remote option available, though in-person attendance strongly recommended.

Successful Outcome:

- Consistent attendance from at least two faculty members in mathematics and at least two faculty members in MLD / CS.
- Consistent attendance from at least three graduate students or postdocs in MLD and at least three graduate students or postdocs in mathematics.
- At least one collaborative research project is sparked between mathematics and MLD/CS based on papers read in the group.

Topics

Neural Operators

Questions

- What problems do neural operators enable us to solve that we can't solve with traditional techniques?
- How can we adapt neural operators to more complex geometries, and how can we use them in regimes where it's already hard to solve the underlying PDE (and hence where there is little training data)?

Papers

- https://arxiv.org/abs/2010.08895
- https://arxiv.org/abs/2108.08481

Foundation Models

Questions

- How can we use techniques for large-scale training of neural networks to improve scientific applications of neural networks?

Papers

- *https://arxiv.org/abs/2403.07187*
- *https://arxiv.org/pdf/2405.19101*

Fluids

Papers

- *https://www.annualreviews.org/content/journals/10.1146/annurev-fluid-010719-060214*
- *https://www.nature.com/articles/s43588-022-00264-7*
- *https://arxiv.org/abs/2201.06780*
    - *https://www.quantamagazine.org/deep-learning-poised-to-blow-up-famed-fluid-equations-20220412/*

Homogenization / Multiscale Methods

Questions

- How can neural networks help accelerate multiphysics simulations?

Papers

- https://arxiv.org/abs/2306.12006
- https://arxiv.org/abs/2102.07256
- *https://arxiv.org/abs/1912.02968*
- *https://arxiv.org/abs/2309.10933*

Complex Geometries

Questions

- *Can grid-free methods based on neural networks simplify PDE simulations defined over complex and irregular domains?*

Papers

- *https://www.sciencedirect.com/science/article/abs/pii/S0952197623015087*
- https://pubs.aip.org/aip/pof/article/33/2/027104/1065963/A-point-cloud-deep-learning-framework-for

Physics-Informed Neural Networks

Questions

- When can PINNs be used to solve equations that we can't solve otherwise? What do they make simpler?
- What accuracy can we expect from PINNs? Can we get the accuracy to something reasonable for applied mathematicians – say, single precision?
- What neural network architecture should we use for PINNs?

Papers

- *https://www.osti.gov/pages/servlets/purl/2282016*
- *https://www.sciencedirect.com/science/article/abs/pii/S0021999118307125*
- *https://www.osti.gov/biblio/2281727*
- *https://asmedigitalcollection.asme.org/heattransfer/article/143/6/060801/1104439*
- *https://arxiv.org/abs/1906.01170*
- *https://arxiv.org/pdf/2105.09506*

Hybrid Approaches

Questions

- *How can machine learning be combined with traditional solvers (rather than replace them) to combine the benefits of both approaches?*

Papers

- *https://arxiv.org/abs/1808.04930*

Diffusions and Generative Models for Science

Questions

- What novel applications are there for generative models in the sciences, besides traditional applications to molecular design, drug discovery, etc?

Papers

- https://arxiv.org/abs/2302.07400v2
- https://arxiv.org/abs/2303.08797
- https://arxiv.org/abs/2403.13724

Statistical Mechanics

Questions

- *Can we solve high-dimensional Fokker-Planck and committor equations using machine learning?*
- *Can we compute rare events in statistical mechanical systems using machine learning?*
- *Can neural network approaches accelerate (read: make possible) nonequilibrium control?*
- *What neural network architecture should we use to represent interacting particle systems?*
- *Can we use foundation model-type approaches to generalize across distinct particle systems, and will this help improve accuracy? Will this aid applications to low-data regimes such as experimental systems?*

Papers

- *https://www.cambridge.org/core/journals/european-journal-of-applied-mathematics/article/abs/solving-parametric-pde-problems-with-artificial-neural-networks/6D3B9A9B9F5F99F4E7D633A9E01ED9FF*
- *https://link.springer.com/article/10.1007/s40687-018-0160-2*
- *https://proceedings.mlr.press/v145/li22a.html*
- *https://journals.aps.org/pre/abstract/10.1103/PhysRevE.105.024115*
- *https://www.pnas.org/doi/abs/10.1073/pnas.2318106121*
- *https://arxiv.org/abs/2206.04642*

Computer Graphics

Questions

- *Many PDEs arise in computer graphics, where the goal is visual fidelity rather than scientific accuracy. Can we develop neural network approaches that achieve this goal rather than scientific accuracy?*
- *Because computer graphics is part of the CS community, they have been quicker to adopt neural network-based techniques than applied mathematicians. Can we take inspiration from their approaches and bring them to the scientific computing domain?*

Papers

- *https://arxiv.org/pdf/2405.15891*
- *https://proceedings.neurips.cc/paper_files/paper/2021/file/810dfbbebb17302018ae903e9cb7a483-Paper.pdf*
- *https://dl.acm.org/doi/abs/10.1145/3326362*

Quantum Mechanics

Questions

- *Are there generative modeling-based techniques that can accelerate quantum Monte Carlo (QMC)?*

- *What neural network architecture should we use for representing quantum states?*
- *Can foundation model-type approaches help here?*

Papers

- *https://www.science.org/doi/abs/10.1126/science.adn0137*
- *https://arxiv.org/abs/2305.19685*
- *https://arxiv.org/abs/2211.13672*