Foundational Background of Physically Informed Deep Learning

Radu Balan

University of Maryland
Department of Mathematics and the Norbert Wiener Center
College Park, Maryland *rvbalan@umd.edu*

November 2, 2022
Panel Session 5: Physics Informed AI and Applications to PHM Panels
PHM 2022

Acknowledgments

This material is based upon work partially supported by the National Science Foundation under grant no. DMS-2108900 and Simons Foundation. "Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation."

Collaborators:

Paul Bogdan (USC), Chris Dock (UMD/Tufts), Naveed Haghani (APL), Gaurav Gupta (USC/Google), Sahil Sidheekh (UTD), Tushar Jain (NYU), Maneesh Singh (Verisk/Motive), Xiongye Xiao (USC)

Works:

1. N. Haghani, M. Singh, R. Balan, *Graph Regression and Classification using Permutation Invariant Representations*, AAAI 2022.
2. G. Gupta, X. Xiao, R. Balan, P. Bogdan, *Non-Linear Operator Approximation for Initial Value Problems*, ICLR 2022.
3. S. Sidheekh, C. Dock, T. Jain, R. Balan, M. Singh, *VQ-Flows: Vector Quantized Local Normalizing Flows*, UAI 2022.

How Physics Inspire AI Solutions

Artificial Intelligence has widespread applications, from autonomous navigation, to security systems, to e-commerce, to machine monitoring (PHM), etc.
Modeling Principles that aid in Machine Learning design:

1. IC/BV Problems: When you know the Differential Equation problem, use it for training via automatic differentiation: **P**hysics-**I**nspired **N**eural **N**etworks[1]
2. Input-Output Operators: If you know that dynamics is simpler in a transformed domain, use pre-/post-transforms: **F**ourier **N**eural **O**perators[2] ; **M**ulti-**W**avelet **N**eural **O**perators[3].
3. Conservation Laws and Invariants: If you know certain conservation laws, use them to design your network: Dissipative SymODEN[4]; if you know the outcome should be invariant to certain transformations, build an architecture that satisfies that invariance: Permutation Invariant GNNs[5]

[1] M. Raissi, P. Perdikaris, G.E. Karniadakis, arXiv:1711.10561
[2] Li, Kovachki, Azizzadenesheli, Liu, Bhattacharya, Stuart, Anandkumar, ICLR 2021
[3] G. Gupta, X. Xiao, R.B., P. Bogdan, ICLR 2022
[4] Y. Zhong, B. Dey, A. Chakraborty: arXiv:2002.08860
[5] N. Haghani, R.B., M. Singh: arXiv:2203.07546

PINNs

An Example

Results taken from Jiajiang Guan & Howard Elman (UMD AMSC663/664 2021 project report)

Train a NN or PINN to produce solutions of the 1D BV-problem:

$$-\varepsilon u'' + u' = 1 \quad , \quad 0 < x < 1$$
$$u(0) = u(1) = 0$$

Exact solution:

$$\hat{u}(x) = x - \frac{exp\left(-\frac{1-x}{\varepsilon}\right) - exp\left(-\frac{1}{\varepsilon}\right)}{1 - exp\left(-\frac{1}{\varepsilon}\right)}$$

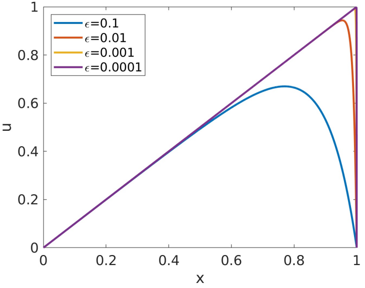


Figure: Exact solution for varying ε

A PINN Example

Its Shortcomings

Train a PINN with the loss function:

$$J(w) = \frac{1}{2N_f}\sum_{k=1}^{N_f} |-\varepsilon u'' + u' - 1|^2|_{x_k} + \frac{1}{2N_b}\sum_{j=1}^{N_b} |u(0)|^2 + |u(1)|^2$$

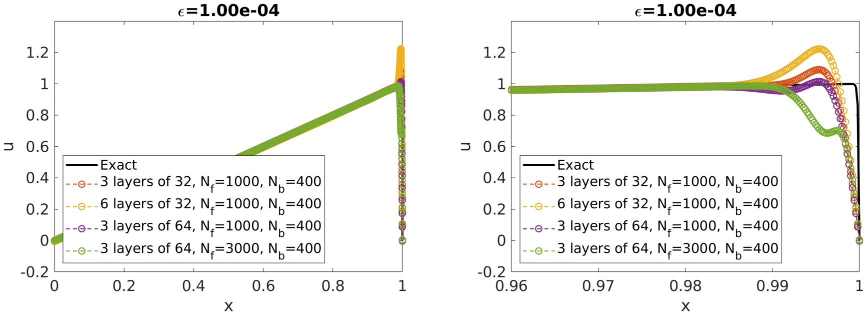


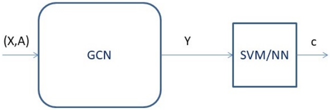
Figure: Approximations done by different network architectures compared to the exact solution; right plot: zoom into the left plot around 1 (credit: Jiajiang Guan).

Invariance and Conservation Laws

Group Invariance or how math can help

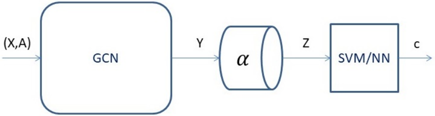
QM9 Dataset: Consists of about 134,000 isomers of organic molecules made up of CHONF, each containing 10-29 atoms[6] Nodes corresponds to atoms; each feature vector containins geometry (x,y,z coordinates), partial charge per atom (Mulliken charge), and atom type.
Task: the task is regression: predict a physical feature (electron energy gap $\Delta\varepsilon$) computed for each molecule.

A "standard" Graph Deep Learning architecture:



$GCN(PX, PAP^T) = GCN(X, A)$: equivariant

A "smarter" architecture:

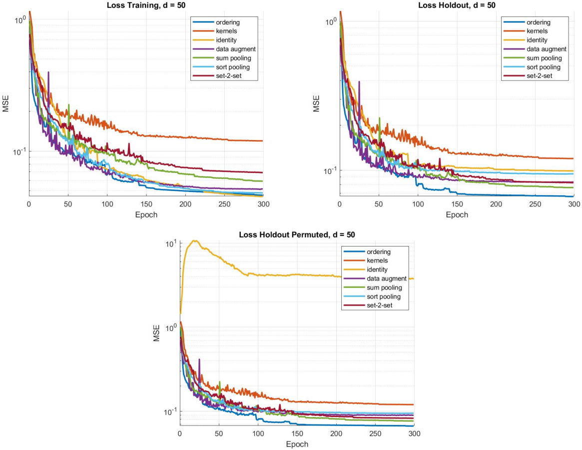


$\alpha(PY) = \alpha(Y)$: invariant to permutations

[6] http://quantum-machine.org/datasets/

QM9 Regression Examples

The following results use "standard" ("identity") mapping and certain permutation invariant mappings[7]:



[7] N. Haghani, R.B., M. Singh: arXiv:2203.07546

Conclusions

... Or next steps?

- Principles of Physics can and should help in designing AI solutions.
- We have exploited some low-hanging fruits.
- There are still other immediate solutions waiting for applications.
- However there are also many open questions/problems hat remain to be solved.

QUESTIONS?