Physics-Guided Machine Learning for Scientific Knowledge Discovery

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Motivation

- We aim to build new physics-guided machine learning methods that leverage complementary strengths of physics and machine learning
  - Physics-based (mechanistic) models uses approximations and imperfect parameterization and thus are approximations of reality.
  - Machine learning methods often require large training data and also cannot generalize to out-of-sample scenarios.

Project Description

- We will explore new methods to integrate physical knowledge into machine learning
  - New deep learning architectures that naturally incorporate relationships amongst physical variables
  - New learning strategies that can leverage physical simulations
  - Implement algorithms for monitoring water temperature in Delaware River Basin

Promise

- Initial results: incorporating physics into an RNN model can significantly improve the predictive model given limited training samples

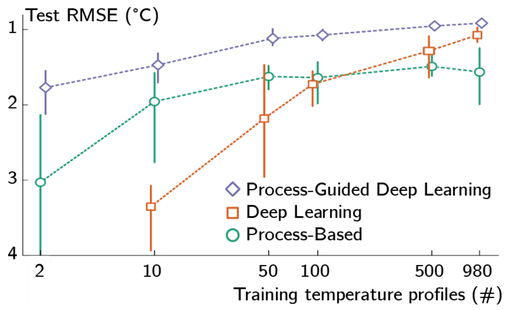

Figure: Physics-guided deep learning outperforms both process-based and blackbox deep learning approaches for predicting lake water temperature, across the entire range of training temperature profiles

- Can we build new deep learning architectures that reflect relationships amongst modular or functional components in physics-based models?
- Can we better leverage physical simulations?

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Advancing **Deep Learning** by Leveraging **Physical Knowledge** for Scientific Discovery

Project Deliverables

- New deep learning architectures that integrate interactions amongst rivers, climate, and reservoirs in Delaware River Basin.
- The proposed method can be widely applied to a broad range of scientific problems where physics-based models are being used.
- We will publish our methods and results in data mining and AI conferences.
- We will also work with government agencies to apply proposed methods for predicting water temperature in large-scale river networks.

Potential Impact

- This project, if successful, will advance existing machine learning algorithms to be better suited for scientific problems.
- This research will have a broad reach and will contribute to real-world problems of great societal needs.

References and/or Acknowledgements

- Willard, J., Jia, X., Xu, S., Steinbach, M., & Kumar, V. (2020). Integrating physics-based modeling with machine learning: A survey. arXiv preprint arXiv:2003.04919.