MACHINE LEARNING FOR FORECASTING AND CONTROLLING ACTIVE NEMATICS

Phu Tran[1], Aparna Baskaran[1], Michael Hagan[1], Pengyu Hong[2], Seth Fraden[1]
[1]Deparment of Physics and [2]Department of Computer Science, Brandeis University

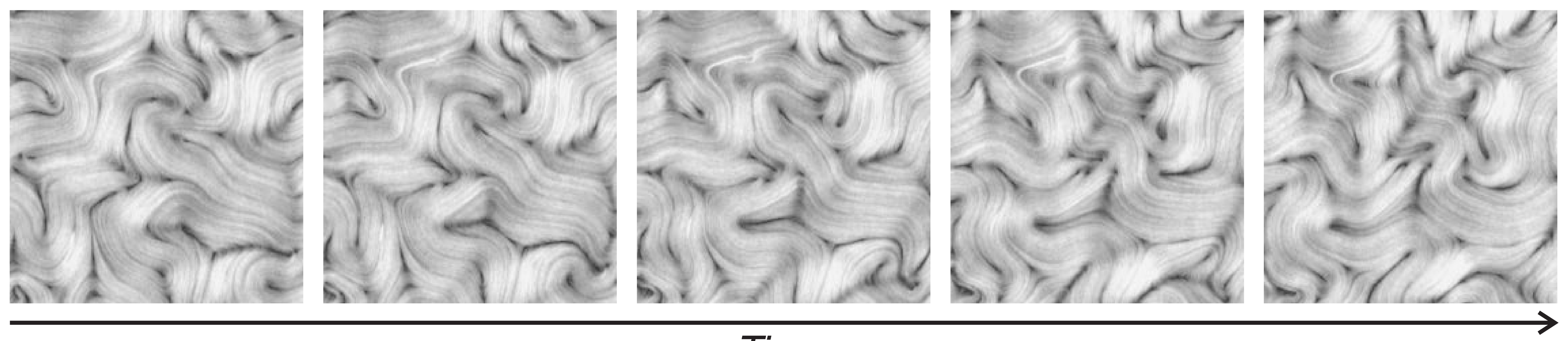
2022 Annual MRSEC Retreat (March 23rd, 2022)

MOTIVATION

- Modern deep learning is very successful in solving practical and challenging problems, e.g., protein structure prediction, drug discovery, self-driving car, unsupervised machine translation, etc.
- Data-driven models is an important approach when mathematical modeling becomes extremely challenging.
- Well-designed physics-informed machine learning models could assist theory discovery.

FORECASTING ACTIVE NEMATICS

- Dynamics of active nematics by a sequence of images



- Respective local orientation of microtubules over time

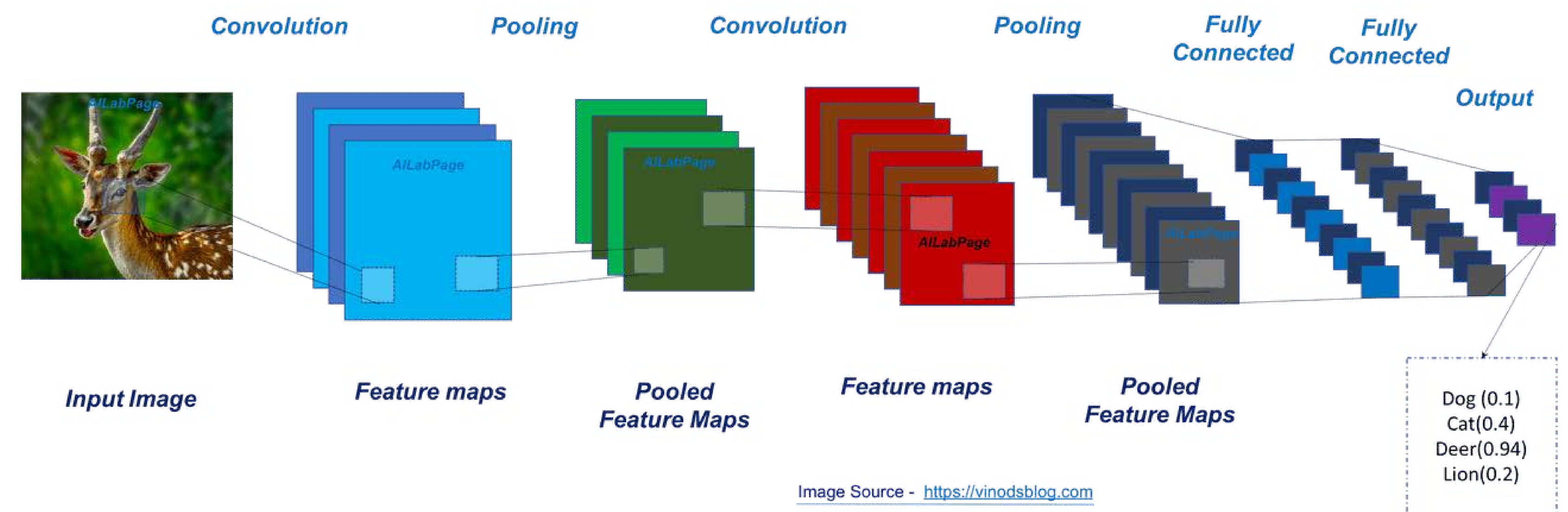
Pixel intensities indicate local orientation of MTs: Black (**0** deg) to White (**180** deg)

RESEARCH PROBLEMS

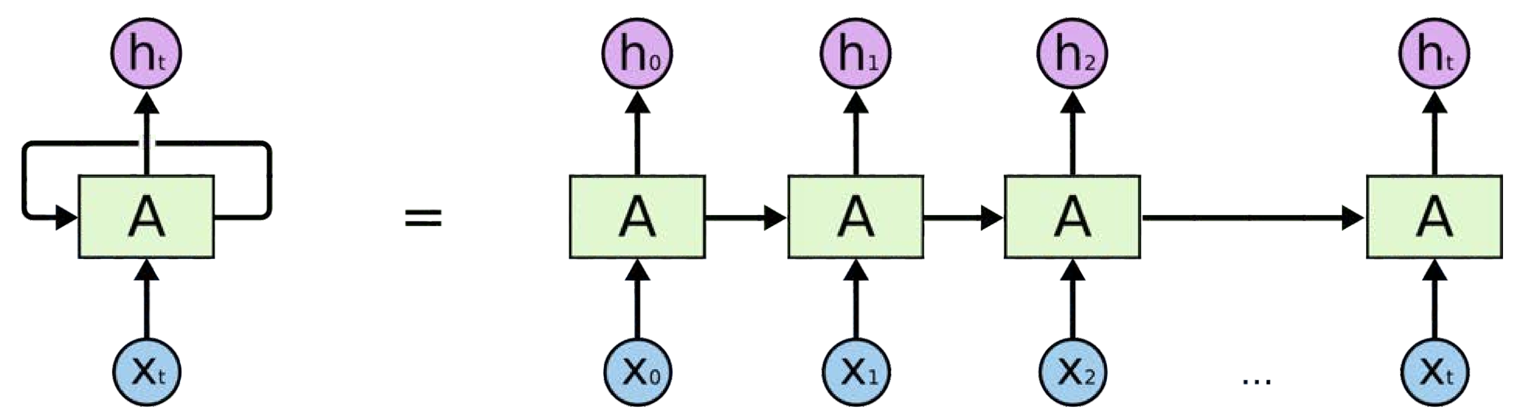
- Data-driven model to predict future states of the system, e.g., predict future sequence (images) given a recent sequence
- Better generalization (i.e., require minimal re-train when applied on different datatsets)
- Interpretability (physically explainable)
- Extendable in control problem (later phase of the project)

DEEP LEARNING

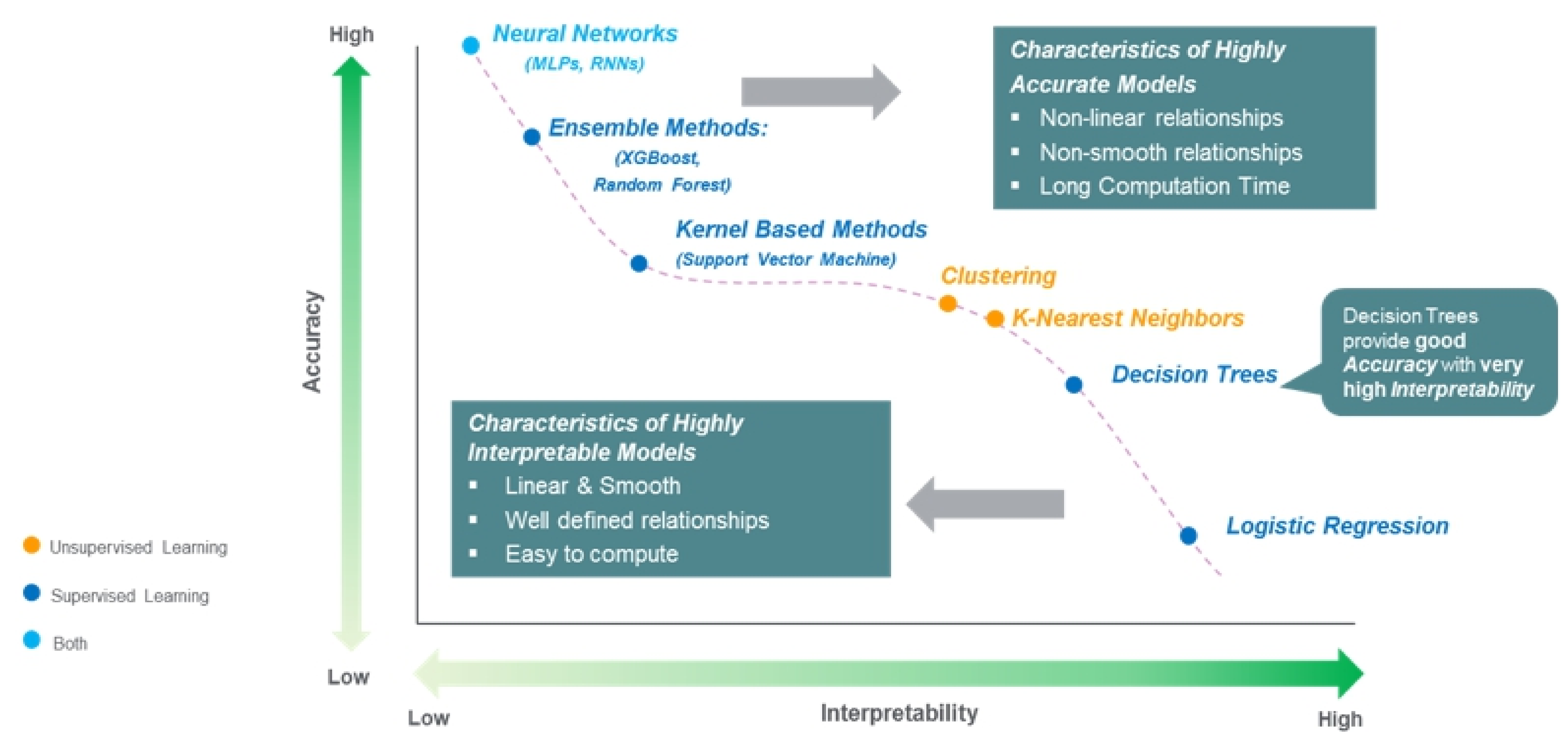
Convolutional Neural Network for Learning Spatial Patterns



Recurrent Neural Network for Learning Temporal Dynamics



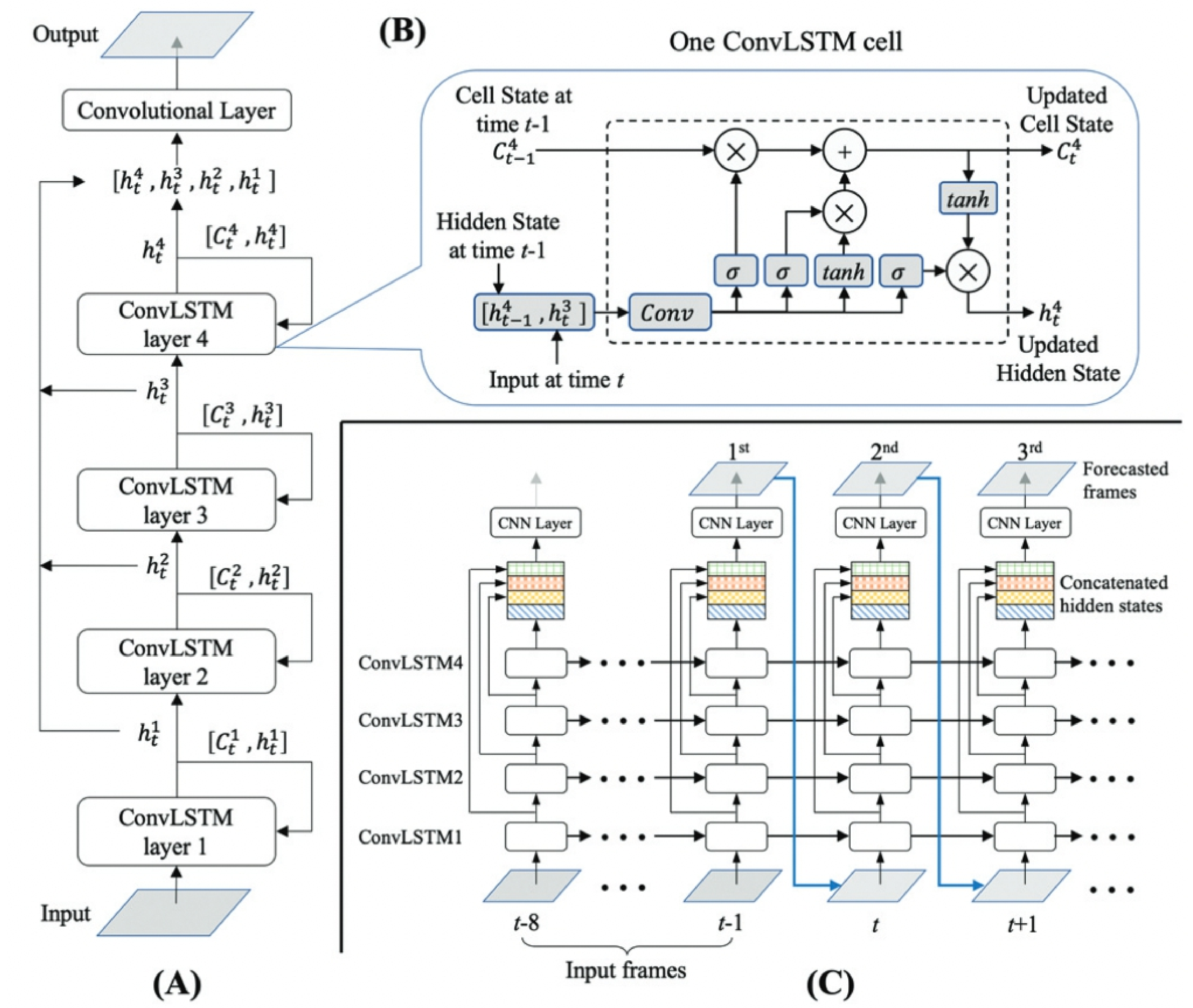
Accuracy vs. Interpretability

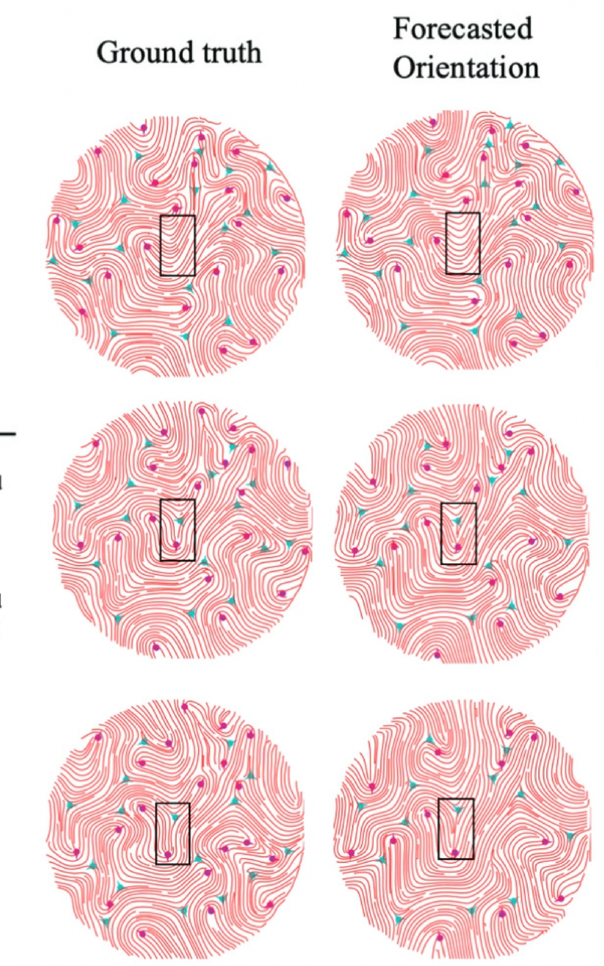


Towards physics-informed model

- Perform data augmentation using domain knowledge in physics
- Design specific network architectures that imitate certain physical properties of the system
- Include well-known physics constraints in the loss function used to train the model's weights

RELEVANT WORK





CURRENT APPROACHES

- The transition from an image to the next one is generally complex (high dimensional and high degrees of freedom)
- Project the images to some latent space such that the dynamics in the latent space is less complex than that in the original one
- Try to integrate physical time and space derivatives into the recurrent neural network architecture
- Current tasks: data gathering and analysis, representation learning

ACKNOWLEGEMENT

We acknowledge support from the DOE (DE-SC0022291), the Brandeis Center for Bioinspired Soft Materials, and NSF MRSEC (DMR-2011846). We also acknowledge computational support from NSF XSEDE computing resources allocation TG-MCB090163 (Stampede and Comet) and the Brandeis HPCC which is partially supported by the NSF through DMR-MRSEC 2011846 and OAC-1920147.

REFERENCES

G. E. Karniadakis et al., "Physics-informed machine learning," Nat Rev Phys, vol. 3, no. 6, Art. no. 6, Jun. 2021, doi: 10.1038/s42254-021-00314-5.

Z. Zhou et al., "Machine learning forecasting of active nematics," Soft Matter, vol. 17, no. 3, pp. 738–747, 2021, doi: 10.1039/D0SM01316A.

Contact: phutran@brandeis.edu