Bridging AI and Domain-science Communities

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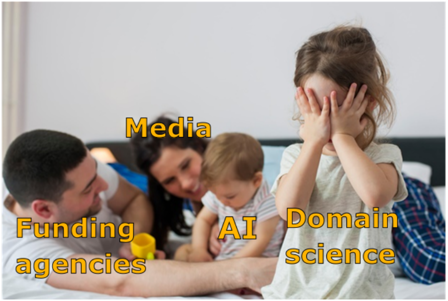
Motivation



How do we get from here?

image sources: wisebread.com, parent24.com

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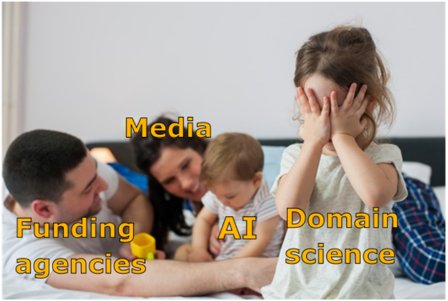

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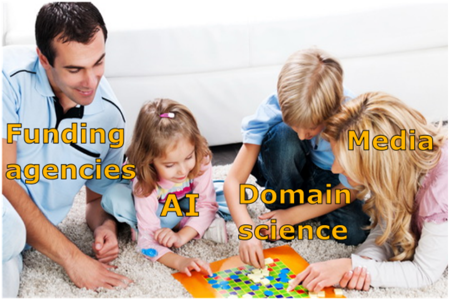

To Here.

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Machine Learning Success Stories and Fails

Success stories in virtual and static environments

- Convolutional neural networks (CNNs) revolutionized image processing
- Long-short term memory (LSTM) networks revolutionized natural language processing
- Deep Reinforcement Learning (RL) achieves superhuman score in Atari games
- AlphaGO beats human champion in the game Go

Fails in real-world dynamic environments[1,2]

- Learning on the real dynamical systems from limited data.
- Problems with overfitting and generalization.
- No guarantees on safety and constraints satisfaction.
- Lack of explainability and interpretability.

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[1] Alex Irpan, Deep Reinforcement Learning Doesn't Work Yet `https://www.alexirpan.com/2018/02/14/rl-hard.html`

[2] Gabriel Dulac-Arnold, Daniel Mankowitz, Todd Hester, Challenges of Real-World Reinforcement Learning, arXiv 2019.

Research Opportunities

	Physics-based	Data-driven	Domain-aware AI
Data efficient	+	-	+
Constraints	+	-	+
Robustness	+	-	+
Model inference	-	+	+
Adaptive models	-	+	+
Scalability/Cost	-	+	+

Definition

Domain-aware AI or Scientific ML are methods and tools for data-driven modeling which respects physical laws and constraints[a] by:

- Incorporating domain knowledge in the model architectures
- Incorporating domain knowledge with auxiliary loss function terms
- Interfacing with physics-based models and scientific computing tools

[a] Gray-box modeling is early-stage domain-aware AI.

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Literature Samples on Scientific ML

- **Domain-aware architectures:** Ricky T. Q. Chen, et al., Neural Ordinary Differential Equations, 2018.
- **Implicit layers in neural networks:** A. Agrawal, et al., Differentiable Convex Optimization Layers, 2019.
- **Stable neural architectures:** Haber, Eldad, and Lars Ruthotto. Stable architectures for deep neural networks. 2017.
- **Domain-aware loss functions:** M Raissi, et al., Physics Informed Deep Learning (Part I): Data-driven Solutions of Nonlinear Partial Differential Equations, 2017.
- **Differentiable programming:** Innes, Mike, et al. A differentiable programming system to bridge machine learning and scientific computing. 2019.

Bottom line: Borders between ML and physics models are getting blurred.

ML for Control in the Buildings Domain

- **Best paper award at BuildSys 2019:** Chen, Bingqing and Cai, Zicheng and Bergés, Mario, Gnu-RL: A Precocial Reinforcement Learning Solution for Building HVAC Control Using a Differentiable MPC Policy, BuildSys 2019. `https://github.com/INFERLab/Gnu-RL`
- **ESTC best paper award at DSCC 2020:** Jan Drgona, Lieve Helsen, Draguna Vrabie, Cutting the Deployment Costs of Physics-based MPC in Buildings by Simulation-based Imitation Learning, DSCC 2020.
- **100+ citations in a single year:** J.R. Vazquez-Canteli, and Z. Nagy, Reinforcement learning for demand response: A review of algorithms and modeling techniques, Applied Energy, 2019.
- **Latest review:** Anjukan Kathirgamanathan, Mattia De Rosa, Eleni Mangina, Donal P. Finn, Data-driven predictive control for unlocking building energy flexibility: A review, Renewable and Sustainable Energy Reviews, 2020.
- **Current efforts at PNNL:** Jan Drgona, Aaron Tuor, Draguna Vrabie, Constrained Physics-Informed Deep Learning for Stable System Identification and Control of Unknown Linear Systems, arXiv, 2020. `https://github.com/pnnl/deps_arXiv2020`

Bottom line: ML for control is getting traction in the buildings domain.

ML for X in the Buildings Domain

- **Energy Use Forecasting:** Felix Bünning, Philipp Heer, Roy S. Smith, John Lygeros, Improved day ahead heating demand forecasting by online correction methods, Energy and Buildings, 2020.
- **Energy performance evaluation:** Saptarshi Bhattacharya, Yan Chen, Sen Huang, Draguna Vrabie, A Learning-based Time-efficient Framework for Building Energy Performance Evaluation, Energy and Buildings, 2020.
- **Occupancy Modeling:** Xin Liang, Tianzhen Hong, Geoffrey Qiping Shen, Occupancy data analytics and prediction: A case study, Building and Environment, 2016.
- **Fault Detection:** J Granderson, G Lin, A Harding, P Im, Y Chen, Building fault detection data to aid diagnostic algorithm creation and performance testing, 2020.
- **Predictive Maintenance:** Min Lin, Afshin Afshari, Elie Azar, A data-driven analysis of building energy use with emphasis on operation and maintenance: A case study from the UAE, Journal of Cleaner Production, 2018,
- **System design:** Nathan C. Brown, Design performance and designer preference in an interactive, data-driven conceptual building design scenario, Design Studies, 2020.
- **Knowledge Transfer:** I. Chakraborty, S. P. Nandanoori and S. Kundu, Virtual Battery Parameter Identification Using Transfer Learning Based Stacked Autoencoder, 17th IEEE International Conference on Machine Learning and Applications (ICMLA), 2018.
- **Cyber security:** Craig Bakker, Arnab Bhattacharya, Samrat Chatterjee, Draguna L Vrabie, Learning and Information Manipulation: Repeated Hypergames for Cyber-Physical Security, IEEE Control Systems Letters, 2019.

Bottom line: ML is versatile and can be combined with existing methods.

Networking, Outreach, and Funding Opportunities

Networking and Outreach:

- Invited talks and workshops at main control conferences: CDC, ACC, ECC.
- Invited talks and workshops at main ML conferences: NeurIPS, ICML, ICLR.
- Climate Change AI workshops[3] and forum[4]. ML community organizing workshops at NeurIPS, ICML, ICLR.
- The American Society of Mechanical Engineers (ASME) Energy Systems Technical Committee (ESTC)[5] organizing workshops and invited sessions at ACC, DSCC.

Funding:

- Department of Energy to Provide $X Million for Artificial Intelligence Research[6].
- EU is increasing its annual investments in AI by 70% under H2020[7].

[3] www.climatechange.ai/

[4] forum.climatechange.ai/

[5] community.asme.org/dynamic_systems_control/w/wiki/16128.energy-systems.aspx

[6] www.energy.gov/articles/department-energy-announces-20-million-artificial-intelligence-research

[7] ec.europa.eu/digital-single-market/en/artificial-intelligence

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[6] www.energy.gov/articles/department-energy-announces-20-million-artificial-intelligence-research

[7] ec.europa.eu/digital-single-market/en/artificial-intelligence

Opportunities for BOPTEST WP1.2

Outreach Challenge

We have cool models! But how to maximize outreach?
What needs to be done for rapid expansion of users and market domination?

BOPTEST Outreach Strategies

- Continue development of compelling web design and visualisations.
- Curated open-source datasets for modeling and forecasting tasks. No need for running the simulations, just download and play.
- Easy setup with AI-user friendly interface, e.g. via OpenAI gym[a].
- AI-focused tutorials and templates. Run by example.
- Problems with different degrees of complexity (leveling up experience).
- Workshop demonstrations at the top AI and control focused conferences: NeurIPS, ICLR, ICML, ACC, CDC, ECC

[a] gym.openai.com

Conclusions

Opportunities

- Open multidisciplinary research topics in domain-aware AI. Team up!
- Funding in on a rise through various agencies like U.S. DOE ASCR, H2020 initiatives.
- Networking and outreach to AI and control communities through invited talks, conferences, workshops, forums, co-authored papers.
- BOPTEST user expansion through easy setup, user friendly interface experience, AI-focused tutorials, open-source datasets, workshop demonstrations.

Pacific Northwest NATIONAL LABORATORY

IBPSA Project 1

U.S. DEPARTMENT OF ENERGY

WP1.2 Discussion Topics

- Q1: How to prevent cheating by using test set data for training?
  A1: Checkbox with accepting the rules statement?
- Q2: How to promote fair comparison of MPC with data-driven controllers?
  A2: Peer-reviewed KPIs? Offline cpu time (hours), memory requirements for implementation (MB), data requirements (days), computing HW used for training/design, use of prior information (e.g., technical sheets)
- Q3: Differentiation in data usage?
  A3: Static data set vs dynamic simulation option for each case?