Applications of Machine Learning in Chemical Engineering

Tutorial 3: Hybrid Modeling

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Agenda

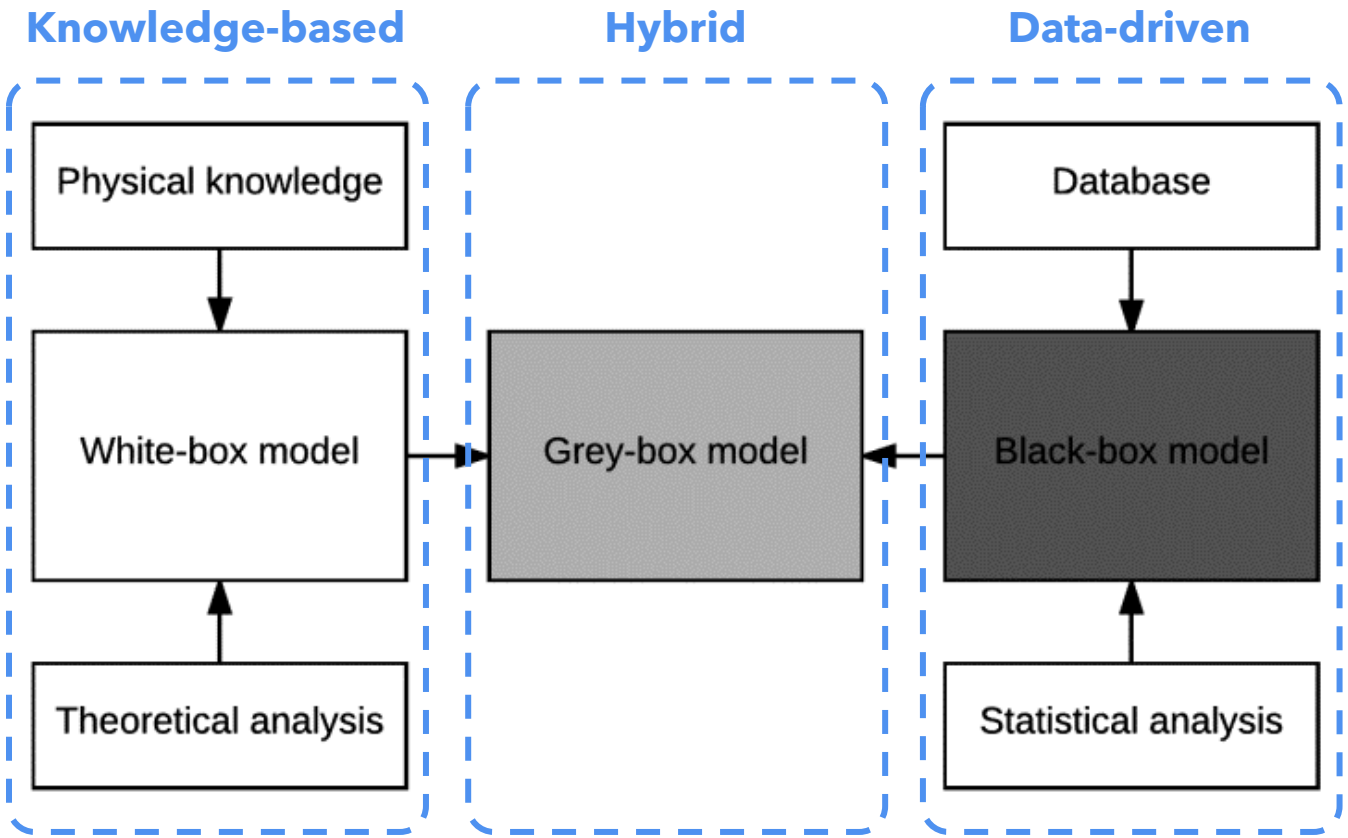
HYBRID MODELING

- Introduction to Hybrid Modeling
- Common architectures of hybrid models:
  - Physics Informed Neural Networks (PINNs)
  - Direct hybrid models (series, parallel, combined)

INTRODUCTION TO HYBRID MODELING

Introduction to Hybrid Modeling

TYPES OF MODELS



Introduction to Hybrid Modeling

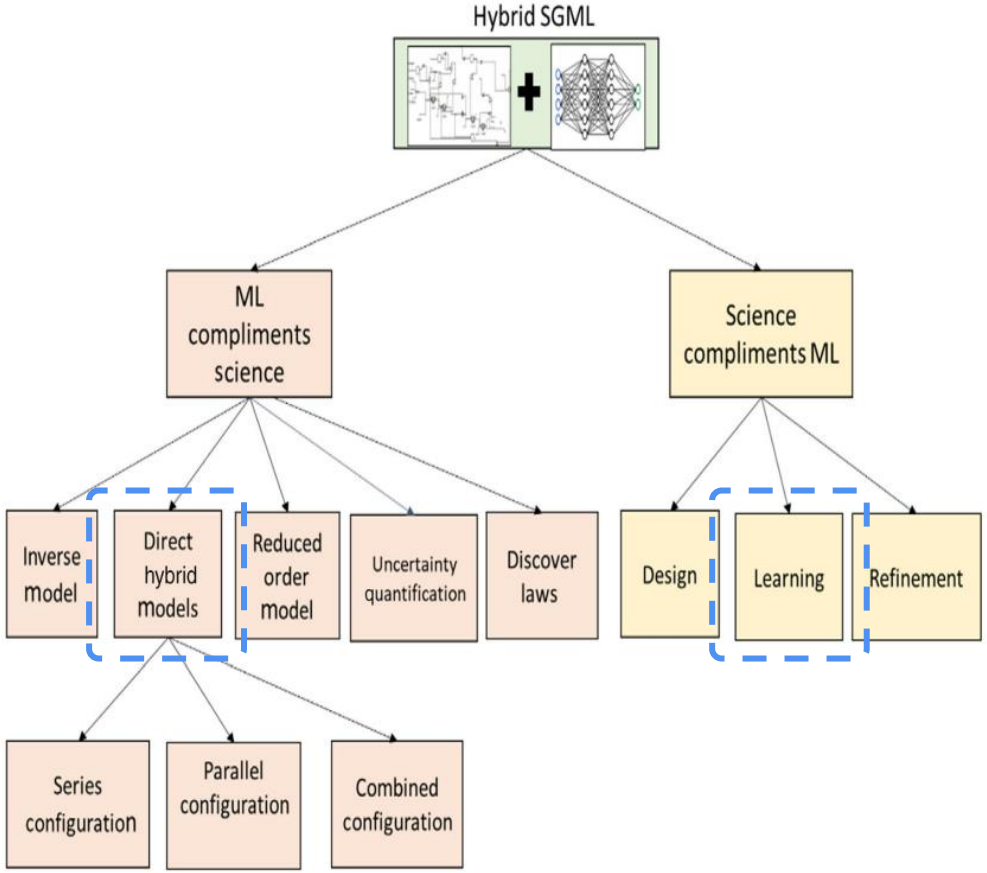
TYPES OF MODELS

Area \ Model	Data-driven	Knowledge-based	Hybrid
Methods	• Machine learning • Statistics	• First principles • Empirical relations	Machine learning & first principles
Dataset size	High	Low	Average
Interpretability	Low	High	High
Generalization	Low	High	High
Prediction accuracy	Higher	Lower	High
Know as	Black-box models	White-box models	• Grey-box • Physics-informed • Science Guided Machine Learning (SGML)

ARCHITECTURES OF HYBRID MODELS

Architectures of hybrid models

CLASSIFICATION OF HYBRID MODELS



Source: Sharma, N., & Liu, Y. A. (2022). A hybrid science-guided machine learning approach for modeling chemical processes: A review. AIChE Journal, 68(5).

Architectures of hybrid models

SCIENCE GUIDED LEARNING

- Scientific principles are used to improve the scientific consistency of data-based models by modifying the machine learning model.

- This is done by incorporating physical relations into any of the following:
  - Loss function
  - Optimization constraints
  - Parameter initialization

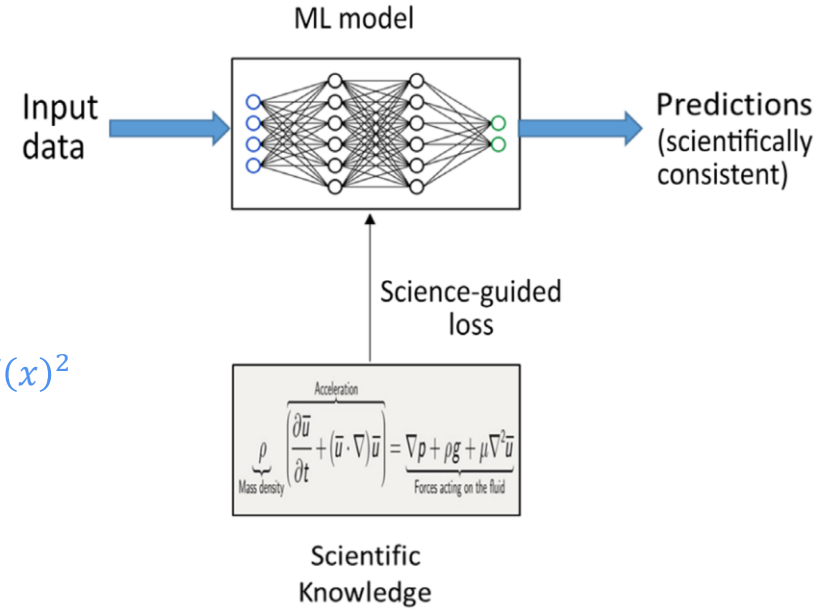
Architectures of hybrid models

PHYSICS INFORMED NEURAL NETWORKS (PINN)

- One of the most common models used for this is the Physics Informed Neural Network (PINN) with science guided loss.
- Loss function is modified to ensure the predictions are consistent with scientific knowledge:

$$L_{total} = L_{data} + L_{physics}$$

$$L_{total} = \frac{1}{n}\sum\left(y_i - y_{pred(i)}\right)^2 + \frac{1}{n}\sum f(x)^2$$



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Architectures of hybrid models

REFERENCES

- Sharma, N., & Liu, Y. A. (2022). A hybrid science-guided machine learning approach for modeling chemical processes: A review. AIChE Journal, 68(5).

Architectures of hybrid models

PHYSICS INFORMED NEURAL NETWORKS (PINN)

- Time to dive into the code:

  https://github.com/SamerHany/CHES307-Applications-of-Machine-Learning-in-Chemical-Engineering/tree/main/Week%203

Thank you

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