Massachusetts Institute of Technology

Robust and expert-agnostic digital twin calibration via ensemble learning and Bayesian optimization

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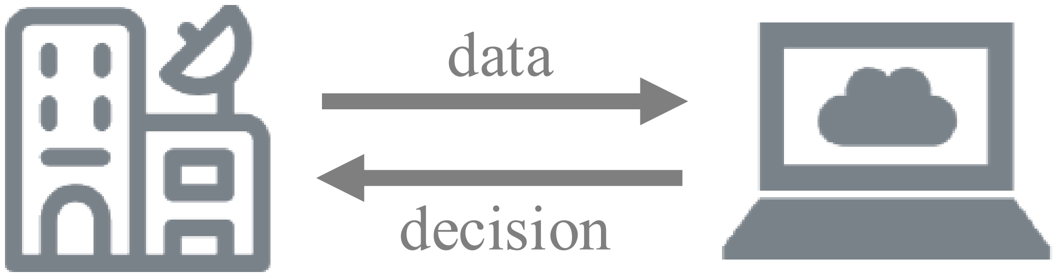
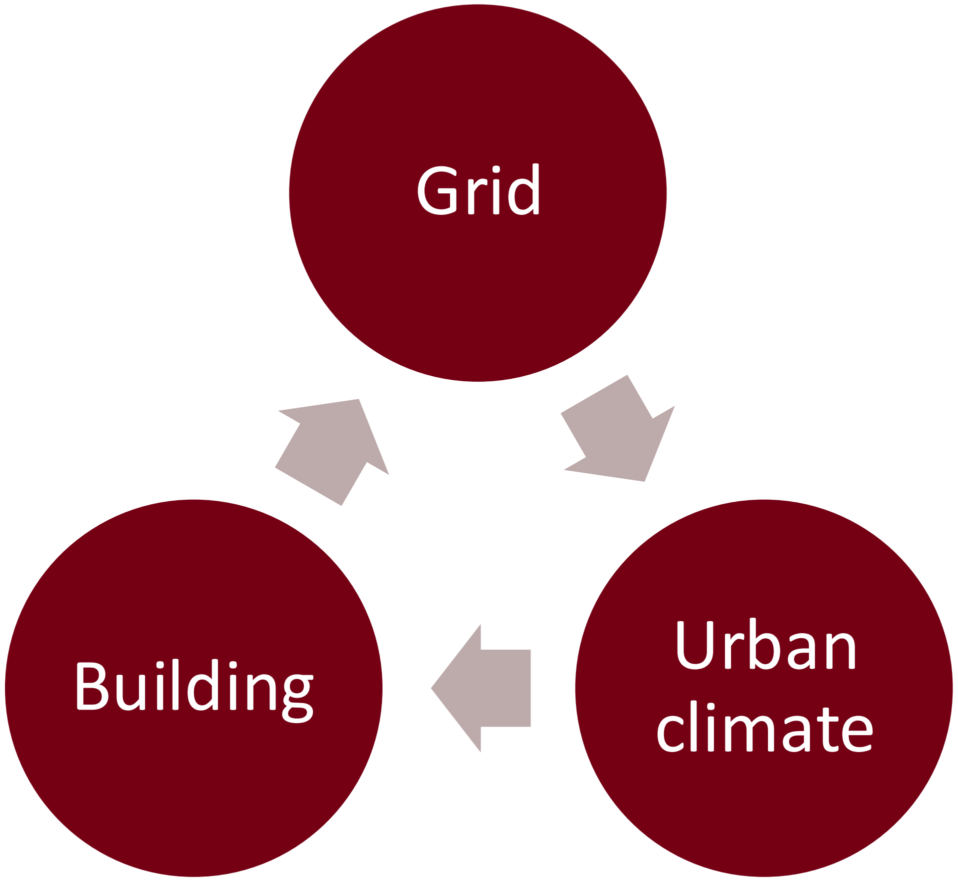
Digital twin applications

Digital twins - Computational models that replicate the behaviour of real-world systems, conducting virtual experiments in unseen scenarios and supporting decision-making

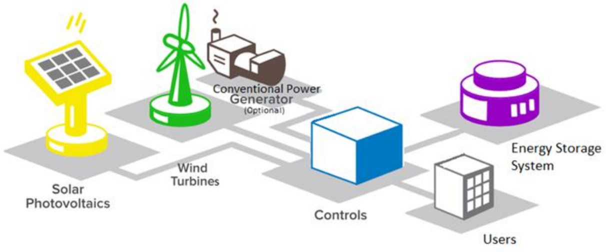




Integrating data and physics

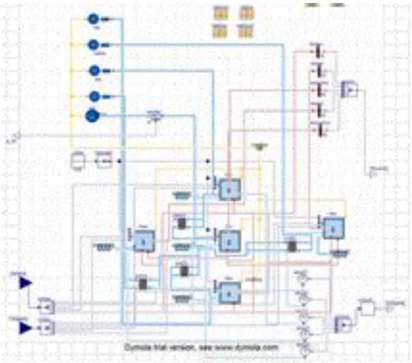
Informed decision-making requires scalable and extrapolatable predictive model

Open complex systems



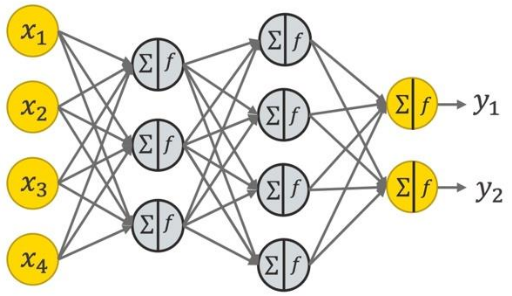
- Heterogeneous dynamics
- Subject to uncertainties
- Under-measured

Physics-based model



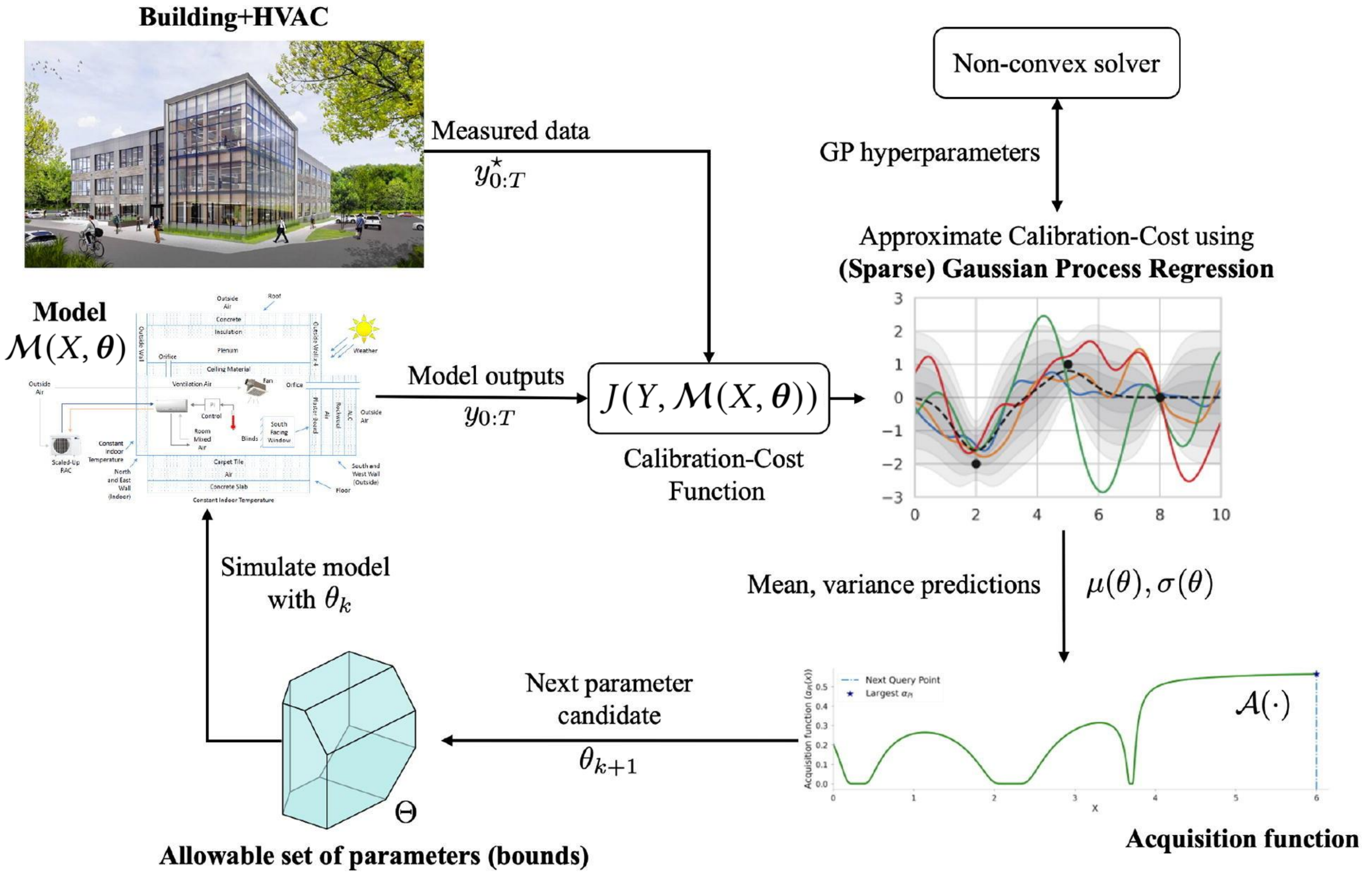
- Extrapolatable
- Low fitting capability
- Unscalable

Fully data-driven models



- High accuracy
- Scalable
- Unreliable in unseen scenarios

Auto-calibration of physics-based models



$$\theta^* = arg \min_{\theta \in \Theta} (J(\hat{Y}, Y))$$

$$s.t. \quad \hat{Y} = \mathcal{M}(X, \theta)$$

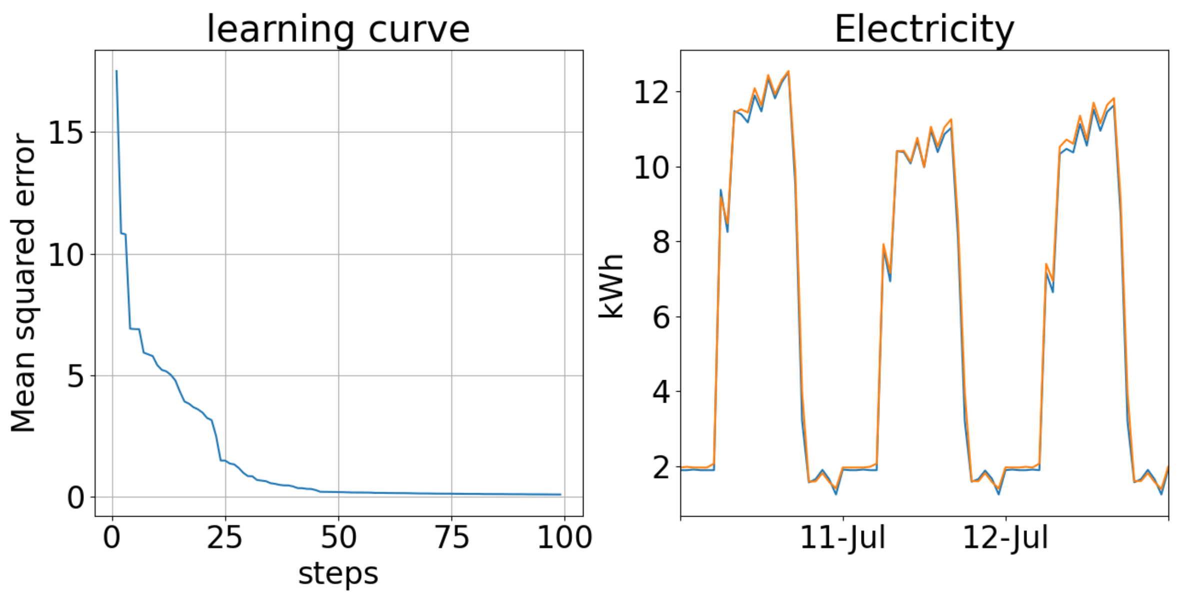
With limited information, how to define the optimization?

- Develop base model
- Obtain X, Y
- Screen parameter

Chakrabarty, A., Maddalena, E., Qiao, H., & Laughman, C. (2021). Scalable Bayesian optimization for model calibration: Case study on coupled building and HVAC dynamics. *Energy and Buildings*, *253*, 111460.

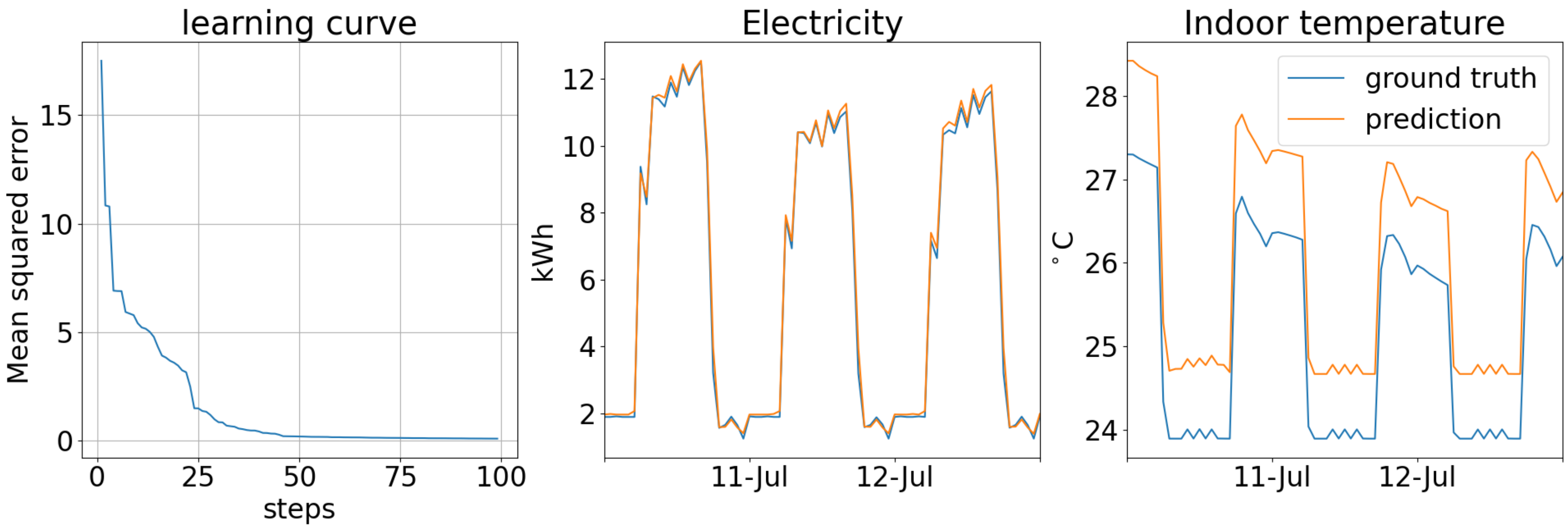
Potential risks in model reliability

- US DOE prototype office building (EnergyPlus, IPCC vs baseline)
  - X: typical meteorological data
  - Y: hourly electricity consumption
  - θ: envelope thermal resistances, outdoor airflow rates, infiltration rates, equipment power densities, solar heat gain coefficients, and cooling setpoints
- Converged after 50 iterations, accurate electricity prediction



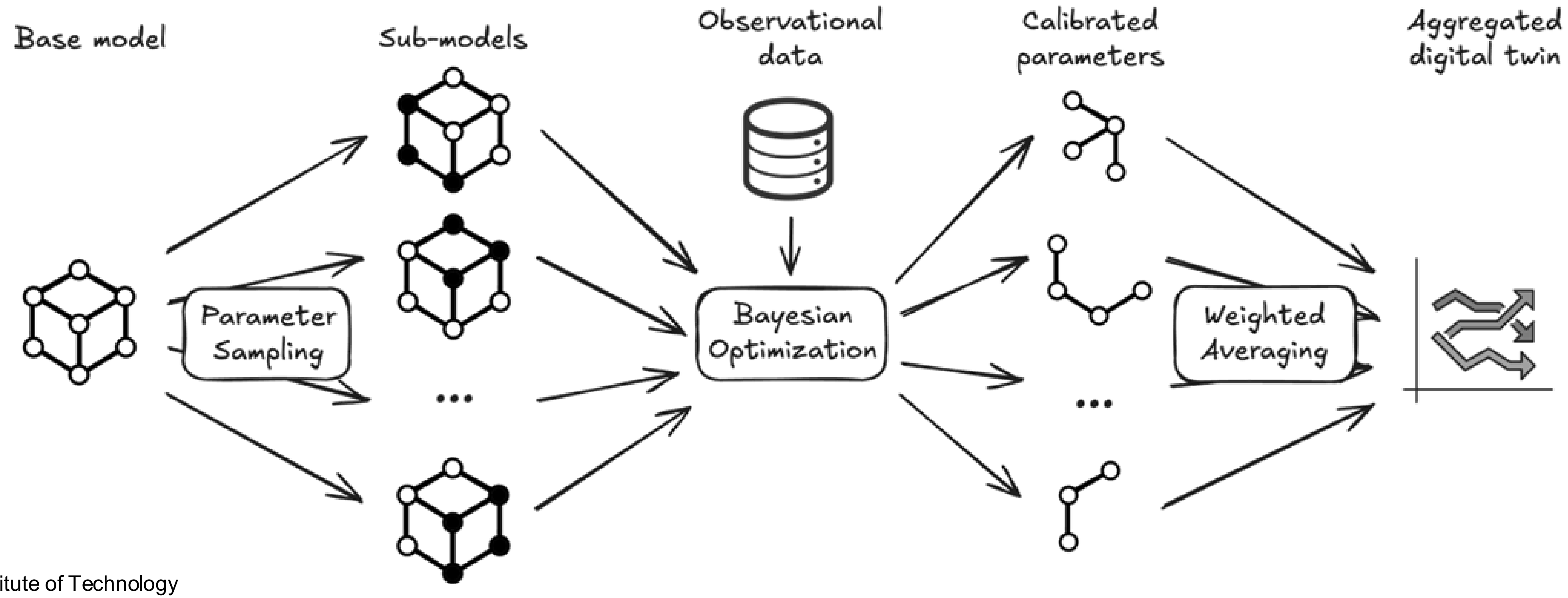
Potential risks in model reliability

- US DOE prototype office building (EnergyPlus, IPCC vs baseline)
  - X: typical meteorological data
  - Y: hourly electricity consumption
  - θ: envelope thermal resistances, outdoor airflow rates, infiltration rates, equipment power densities, solar heat gain coefficients, and cooling setpoints
- Converged after 50 iterations, accurate electricity prediction, but wrong indoor temperature

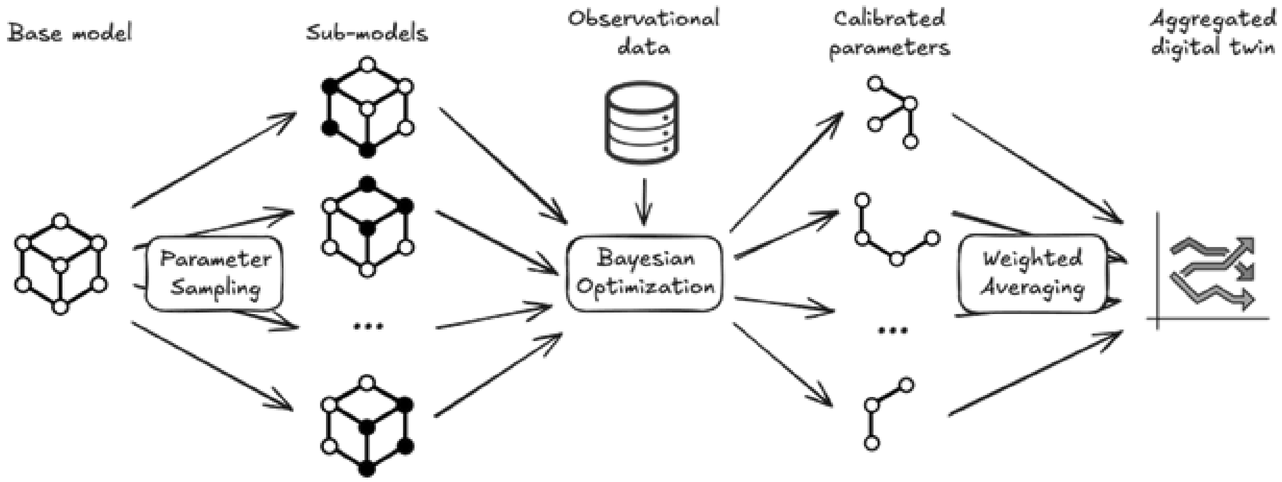


Ensemble learning x model calibration

- Ensemble learning (accurate, but unextrapolatable and uninterpretable)
  - Homogeneous: same model structure, different training dataset
  - Heterogeneous: different model type/structure
- Sub-model development in calibration: randomly sampled parameter sets



Exponentially weighted average



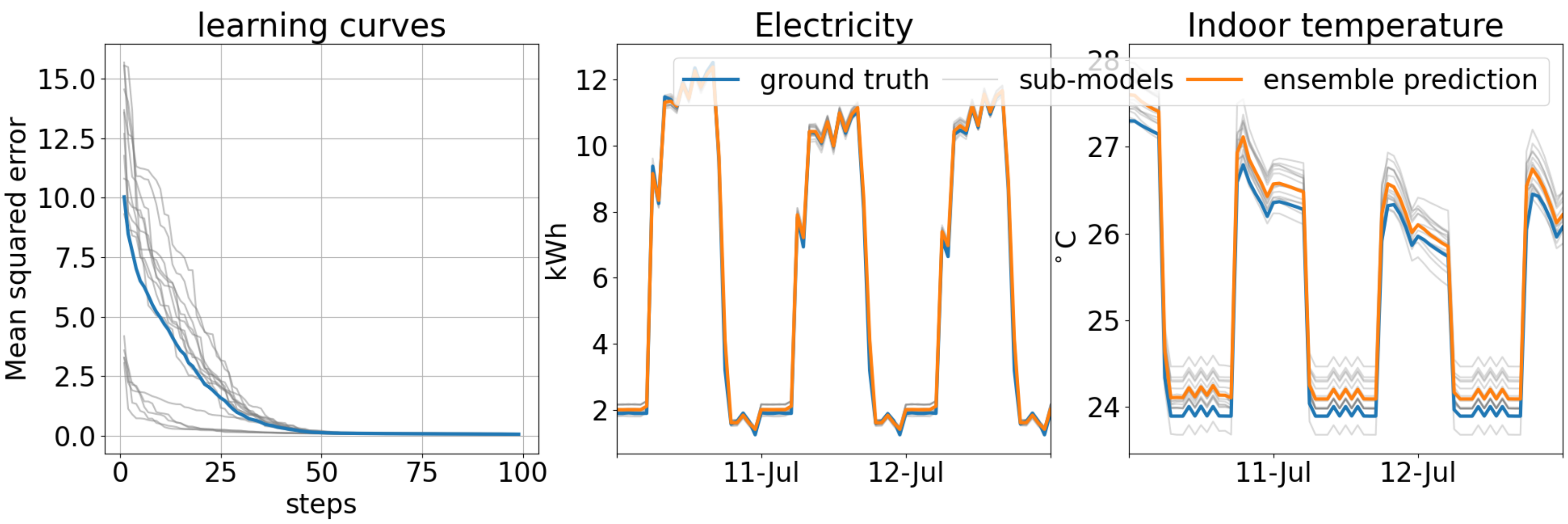
$$\hat{\omega}_j = \frac{\pi_j e^{-\beta \hat{r}_j}}{\hat{\mathcal{L}}}, \qquad j = 1, \cdots, k$$

$$\hat{\mathcal{L}} = \sum_{j=1}^{k} \pi_j e^{-\beta \hat{r}_j},$$

- Weighting factor to quantify the reliability of j_{th} sub-model
  - π: prior distribution on the weight space
  - r: model risk, approximated by mean squared error on validation set
  - β: confidence level on risk estimation

Experimental results

- 15 Sub-models with all possible combinations of four out of the six parameters
- Weighted average of sub-models as the final prediction
  - Similar accuracy to the single calibration on electricity
  - MSE of temperature prediction reduced from 0.74°C to 0.05°C
- Ten times more computational time



Summary

	Black-box ensemble learning	Single physics-based model calibration	Ensemble learned physics-based model calibration
Fitting capability	High	Medium	High
Extrapolation capability	Low	Medium	High
Expert dependency	Low	High	Low
Interpretability	Low	High	High

- Robust digital twin solution for complex and data-scarce open systems
- An additional dimension of heterogeneous ensemble learning, enhancing extrapolatability and interpretability
- While more computational consuming, the calibration process is expert-agnostic
- The aggregated model is not yet ready for control purposes, secondary surrogate model could be useful

Thank you!

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